Review of the Water Quality Model
Analysis and Recommendations of the Scientific and Technical Advisory Committee

The Review

The Implementation Committee requested that STAC undertake a review of the Water Quality Model in the summer of 1988. The Terms of Reference provided by the IC included four specific areas of analysis, all related to the utility of the model for management needs. Recognizing the need to engage highly qualified technical experts in the review and the value of involving reviewers who had no previous experience and opinions about the model, STAC chose to form a Model Review Team (MRT) to conduct the primary review and advise STAC of its findings and recommendations. Most of the evaluations of the MRT fell on a core group, which included three eminent scientists with broad experience in the dynamics of estuarine ecosystems and the development and use of numerical models. Dr. Scott Nixon of the University of Rhode Island, an internationally renowned expert on coastal eutrophication, chaired the MRT.

The MRT Report was presented to STAC on December 9, 1999, at which time it was discussed with the MRT chair. STAC herein submits the independent MRT report as presented and offers its own brief analysis of the issues and specific recommendations.

The Review Process

Although a comprehensive review was not conducted on all aspects of the Water Quality Model, three diagnostic test were preformed to focus on functions and calculations fundamental to the interpretation and prediction of the model in the context of responses of the ecosystem to nutrient loadings and the abatement thereof. Additionally, the MRT evaluated the institutional arrangements for ongoing evaluation of the technical performance of the model.

The STAC believes that the MRT conducted a highly professional and probing review. The MRT report contains a number of highly significant findings and very important recommendations for improving the Water Quality Model and the process by which it has been developed. STAC commends the members of the MRT for an exceptionally thoughtful and valuable evaluation.

The Findings

A number of performance problems were identified in the MRT's diagnostic tests in which model predictions were compared with actual observations of salinity, primary production, respiration and nutrient utilization. These are discussed at length in the MRT report and will not be repeated here.

STAC believes these are serious problems that merit attention in improving the model's ability to predict future conditions. The differences between observations and predictions revealed by the MRT are not trivial. For example, the differences with regard to salinity mean that the physical processes that move and mix materials (ocean and fresh water, nutrients, and organisms) are not yet accurately represented in the model. Nutrient uptake and primary productivity represent the rates by which the nutrients that we are trying to control stimulate the production of organic matter. Respiration rates determine the consumption of oxygen during the processes of production and degradation of that organic matter. These rate variables are fundamental to determining the state variables, such as dissolved oxygen, biomass, and water clarity, used to define water quality. If these rate variables are not accurate one has to question the accuracy of the predictions of the entire Water Quality Model. Even if there is a good match between model predictions and observed state variables, such as dissolved oxygen, placing confidence in predictions of future conditions is difficult if the processes by which they are determined in the model are not accurately depicted. Furthermore, better estimation of such key processes as primary production and respiration is essential for the use of the model to assess consequences to higher trophic levels.

These are significant problems, not scientific fine points representing, as some may suggest, the different perspectives of engineers who develop models for practical purposes and scientists who focus on the unknowns. Engineering is the application of science to achieve practical solutions to everyday problems. Sound engineering and sound model predictions rest on sound science. The MRT's findings indicate that substantially better estimations of important physical and biological processes in the Bay are essential if significant improvements in the predictive capabilities of the Water Quality Model are to be realized. STAC agrees with the MRT that the performance of the model can be substantially improved through better application of scientific knowledge of key biological and physical processes that affect the quality of the Bay.

In addition to issues of model performance, the MRT also found programmatic shortcomings in the integration of the monitoring and modeling programs, communication of clear management goals, irregular or non-existent outside merit review, poor model documentation and inadequate publication in the open, scientific literature. STAC believes that these are important findings that deserve careful reflection and attention by the CBP. STAC itself has frequently noted inadequate connection between monitoring and modeling and has sponsored workshops to improve this situation (e.g. *Integrated Analysis of Chesapeake Bay Monitoring Data*, 1996; *Watershed Response to Changes in Nutrient Loads: The Best Uses of Monitoring and Modeling*, 1997). STAC has also been a steady proponent of critical merit review.

The Use of the Model

The statement in the MRT report that will undoubtedly draw the most attention is: "It is the opinion of this team that the Water Quality Model does not currently provide information suitable for major management decisions and that use of the model for such purposes should be suspended." This reflects the MRT's concerns that there are significant problems with model performance and the observation that these problems were not being taken seriously by CBP modelers. One could react that the MRT overstepped the bounds of a technical assessment in concluding that managers should suspend the use of what they view as a useful, if imperfect, model. Nevertheless, STAC believes the MRT's findings should be understood and embraced as a wake-up call for the technical and management communities broadly involved in the Bay Program to work in a concerted effort to improve the model. This is of particular importance if the model is to be used to establish TMDL target settings over the next year or two.

Do the shortcomings revealed by the MRT evaluation mean that previous applications of the model by managers are unfounded? STAC does not believe they do. An earlier version of the Water Quality Model was used in the 1997 re-evaluation to estimate future dissolved oxygen conditions in response to source reductions. In essence, these results indicated that although dissolved oxygen conditions would improve, hypoxia would not be eliminated even under Limits of Technology assumptions. This conclusion is highly unlikely to change with model refinement although we will be able to predict more accurately how much improvement we can expect. More recently, the current version of the model was used to determine source reductions needed to achieve certain water quality goals in the Virginia tributaries. Despite the shortcomings noted by the MRT, the Water Quality Model is responsive to reductions of nutrient inputs in terms of the types and direction of the changes expected, e.g. increased dissolved oxygen and light penetration. The model was useful in demonstrating to decision-makers the linkages between nutrient inputs, water quality and living resources and the relative effects of point source controls among those tributaries. This was helpful in determining where to target efforts. The shortcomings in representing production and respiration make the model less reliable in estimating the amount of source reduction required to achieve specific water quality "endpoints." But, then that is the objective of the TMDL process that will be a central goal of CBP modeling over the coming months.

Recommendations

Based on the findings of the Model Review Team, the Scientific and Technical Advisory Committee makes the following recommendations:

1. Comprehensive and timely documentation in the scientific literature of the Water Quality Model inputs, calculations, assumptions, and codes should be undertaken immediately. This will allow for external assessment and understanding of the model as well as provide confidence by all users of model outcomes.

2. The Chesapeake Bay Program is encouraged to communicate clear management goals for the use of the Water Quality Model. This will assist in efficient model development and allow prioritization of tasks over the long term.

3. Strategic planning and the exchange of information between the monitoring and modeling programs within the CBP should be instituted, perhaps through restructuring of the subcommittees.

4. Monitoring data should be used in regular verification evaluations of model performance. This will greatly improve the accuracy of the model inputs, as well as

model outputs and concurrently assist in establishing monitoring program priorities and limitations.

5. A comprehensive evaluation of the Water Quality Model should be undertaken as recommended by the MRT. Concurrent with this evaluation, a series of workshops should be held to focus on specific questions and problems identified by the MRT's evaluation. The STAC is willing to assist in the organization of these workshops.

6. Similar evaluations should be conducted in a timely fashion on all modeling efforts of the CBP. Such evaluations will assure that sound, scientific basis for Bay restoration and management are being implemented.

7. Concurrent with recommendation 5, a symposium should be held to investigate alternative modeling approaches for the future. The STAC is willing to assist in the development of such a symposium.

8. Finally it is STAC's assessment that the CBP would benefit from establishing stronger ties with the scientific community and should invest in efforts to improve the understanding of all physical, chemical, and biological processes that effect the quality of the Bay. In particular, immediate new efforts should focus on those issues relevant to TMDL concerns.

Review of the Water Quality Model

A Report from the Scientific and Technical Advisory Committee

November 1999

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Executive Summary

In the summer of 1998 the Implementation Committee of the Chesapeake Bay Program requested that the Scientific and Technical Advisory Committee conduct a review of the Water Quality Model.

The Terms of Reference (TOR) consisted of four specific areas for analysis and an accompanying set of eleven associated questions that are contained in the body of this report. The four areas for analysis address in order of priority: the Water Quality Model and its calibration, the model linkages, ways to increase the utility of the model, and the needed improvements to the model. It is significant that all four areas emphasize application of the Water Quality Model to management needs.

Model Review Procedures

To our knowledge, there does not exist an explicit written formulation of Bay Program management needs. This makes it difficult for the model development team and this review team to determine if the needs of management are being met. Lacking such a formulation, we based our opinion on the model performance in selected areas of particular importance to the Chesapeake Bay ecosystem, especially the parts of the model that are fundamental to the proper computations of dissolved oxygen since the model has already been used to relate nutrient inputs to bottom water oxygen concentrations. This is clearly an area where managers wish to use the model.

Summary of Findings

It is the opinion of this team that the Water Quality Model does not currently provide information suitable for major management decisions and that use of the model for such purposes should be suspended. This conclusion is derived from the findings listed below:

Programmatic

1. The Modeling program and the Monitoring program should be more closely coordinated. Measured and modeled data should be collected and analyzed on compatible spatial and temporal scales so that specific challenges can be put to the model and appropriate measures collected for verification. For example, selected site specific simulations and measurements with high vertical and temporal resolutions. There has also been little effort to compare model performance with rate measurements made by independent investigators around the Bay, including such basics as primary production and water column respiration.
2. The culture of the Bay modeling committee has not been one of critical merit review. It is our view that the Model Evaluation Committee, which may have been a critical review group in the past, is not currently able to perform that function. The larger modeling community, both inside and outside of the Bay area, has not had many opportunities to review and comment on the details of the model and the model results.

Model Performance

1. The model overestimates the salinity gradient and underestimates vertical mixing near the bottom in some regions of the Bay, which can significantly affect the filtration rates and the respiration rates of the benthic organisms and dissolved oxygen concentrations (Appendix A).
2. The fundamental processes, primary production and respiration, are significantly underestimated in several areas of the Bay (Appendices B, C), such that the Bay consumes more organic matter and oxygen than it produces, in contrast to the actual Bay system.
3. The modeled primary production in the water column does not reflect the degree of preference for ammonium over nitrate that is believed to be the actual case. This has profound implications for the Bay ecosystem (Appendix C).
4. The fact that the three fundamental areas examined in this review were found to be seriously compromised makes it inescapable that there must be other major errors that provide compensation. We conclude this because the modeling team staff asserts that oxygen simulations produce values that agree with observations in spite of the large errors in computed oxygen production (from photosynthesis) and water column oxygen consumption.

Documentation, Publications and Reviews

1. Documentation of the Water Quality Model and its components is not readily available, making a thorough understanding of the model and a complete review of it not possible.
2. The model has not been sufficiently subjected to peer review through published scientific papers. This is traditionally an important mechanism for reviewing scientific and engineering results and also a method for uncovering new ideas and techniques.

<u>Recommendations</u>

Based upon the findings of the Team, several recommendations are made below:

1. Re-examine the role of the Modeling Evaluation Group and make appropriate changes. Recommendations include three-year renewable term memberships and more written reviews by MEG and ad hoc review teams; also consider a more independent management reporting structure for MEG.
2. Redesign and re-implement the monitoring and modeling programs to function as coordinated mutually supporting elements of the overall Bay Program.
3. Maintain a complete and up-to-date documentation library of model details, validations and results. This would improve communications with all interested groups and would assist in future reviews of the model.
4. Encourage extensive publications in peer-reviewed literature and presentations at scientific meetings.
5. Review and improve several especially important elements of the Water Quality Model, notably primary production, water column oxygen consumption and nutrient recycling, sediment resuspension, the benthic model, the coastal interaction model.

6. Since several areas in the model are in need of more research, take steps to foster more joint efforts between the estuarine research and model research communities and the model applications communities. The workshops being conducted by the Bay Program this summer are an excellent first step, but they emphasized presentations rather than challenges and specific problems.

Review of the Water Quality Model

1.0 Introduction and Terms of Reference

This report is the product of an effort by the Chesapeake Bay Program (CBP) Scientific and Technical Advisory Committee (STAC) to review the current status and utility of the Water Quality Model (WQM) and its contributions to the integrated Chesapeake Bay model. The integrated model includes the Watershed Model (WSM), the hydrodynamic model and several additional water quality and living resource models which are included in or appended to the WQM. In order to assess the linkages and couplings of the WQM to the other models, the other models were considered to a limited extent.

The Terms of Reference (TOR) provided by the Chesapeake Bay Implementation Committee consisted of four areas for analysis and eleven associated questions. The areas for analysis, in the stipulated order of priority, and all the questions are listed on page 7.

2.0 Structure of the Review

2.1 Study History and Approach
In the summer of 1998 the CBP Implementation Committee (IC) requested that the STAC perform a review of the WQM. The study was initiated in the fall of 1998 when the Modeling Subcommittee of STAC selected the team. A plan was developed in November of 1998 and the first team meeting was held in December of 1998. The approach was to compare the WQM results with the observed data and research findings.

2.2 Team Selection and Organization
A list of candidates was proposed at the STAC meeting in September of 1998 and the Modeling Review Team (MRT) was selected in October. After the study had been initiated it was decided to form the team around a Core group, which was largely scientists <u>not</u> directly involved in the Bay Program, and an adjunct group. The Core Group consisted of:

- Dr. Scott Nixon - University of Rhode Island, Chairman,
- Dr. Eileen Hofmann - Old Dominion University,
- Dr. Hugh Ducklow - Virginia Institute of Marine Sciences,
- Dr. Grant Gross, -Chesapeake Research Consortium,
- Dr. Gordon Smith – Chesapeake Research Consortium/Johns Hopkins University, coordinator,

The Adjunct Group was composed of the members of the Modeling Evaluation Group (MEG) and consisted of:

- Dr. William Boicourt - University of Maryland,
- Dr. Jay Taft - Harvard,
- Dr. Wu-Seng Lung - University of Virginia,
- Dr. Kevin Farley – Manhattan College,

- Dr. Richard Wiegert- University of Georgia.

The Team met six times, December 3, 1998, January 12-14, 1999, March 16-17, 1999, April 29,1999, and June 9, 1999, August 27, 1999. The second meeting coincided with the Modeling Subcommittee (MSC) Quarterly Review and some members of the Team attended that meeting. In addition, Dr. Gross attended all meeting of the monthly MSC between November 1998 and November 1999 and Dr. Smith attended all but one. At the team meetings, presentations were given by Carl Cerco (WES), Rich Batiuk (EPA), Lewis Linker (EPA), Rob Magnien (DNR), Mike Fritz (EPA/Living Resources), and Tom Simpson (USDA/Nutrients). Drs. Boicourt and Lung provided very useful perspectives on the model details and the historical development. November 2, 1999 the team along with Dick Jachowski (STAC) met with Bill Matuszeski (EPA), Rich Batiuk (EPA), and Lewis Linker (EPA) to present the final draft of the report.

2.3 Credits and Thanks
The team would like to thank Lewis Linker and Jeff Sweeney for their help in obtaining materials and providing informative presentations at the meetings and to thank Carl Cerco and the MEG members for their contributions. Ms. Tracy Scheffler and Ms. Jaclin Schweigart provided outstanding administrative support and general guidance.

Terms of Reference

1. Evaluate the status of the Phase IV CBP water quality model and its calibration with respect to its ability to meet CBP management needs regarding future conditions, including but not limited to determination of nutrient reduction goals for Virginia tributaries.

Specific questions:

- Has the model incorporated new information and understanding from scientific research?
- Have the model improvements dealt effectively with important limitations of the previous model?
- How well has the model been calibrated and verified by comparing simulations and actual observations, including hydrodynamics, water chemistry, submerged aquatic vegetation, and lower trophic levels?
- How relevant are the parameters predicted by the model to management needs and how reliable are the most relevant predictions?
- How reliable are model predictions of future conditions in contrast with retrospective simulations?

2. Review the linkages and coupling of model components, both within the water quality model and between it and other elements of the integrated CBP model (e.g. the watershed model) to determine the degree to which they meet CBP management needs for the fully integrated model.

Specific questions:

- How sensitive is the water quality model to the performance of watershed, atmospheric and coastal ocean models?
- How realistic and responsive are the linkages among submodels in the Phase IV water quality model (e.g. sediment-water column)?

3. Identify ways to increase the utility of the model and its products to managers, including tributary teams and local government and to the scientific community.

Specific questions:

- How might model results be better communicated to Bay Program and state managers and other stakeholders interested in model prediction on more local scales?
- How might access to and use of the model (and its components) and model outputs by the scientific community be fostered?

4. Identify areas of the CBP model requiring additional development to meet future management needs and those identified in Executive Council Directives or strategic plans of the CBP subcommittees.

Specific questions:

- How might the linkages and couplings among components of the integrated CBP model be improved?
- What are the inputs, rates and states in the water quality model most in need of improved approximation from the perspective of management needs?

3.0 Limitations and Caveats

In the process of conducting this review, several conditions were encountered which very severely limited the ability of the team to do a balanced and in-depth review and made it impossible for them to directly address many of the questions in the TOR. It is important to emphasize, however, that we do feel that we obtained sufficient information to support our most serious criticisms of the model as it is presently constructed. The items listed below are the principal limitations that were encountered

3.1 Management Needs

The emphasis in the TOR has been placed on the utility of the model for management needs. To our knowledge, CBP management has never explicitly stated their needs with regard to model performance or performance criteria. Lacking a clear charge for the priority of information needs and for the required accuracy and precision, it is difficult to judge if the model is sufficient for those needs. For example, how much uncertainty can the managers tolerate in anoxic volume days, acres of SAV, etc?

3.2 Management Applications and Validation

A model adequate for management purposes may not be completely derived from fundamental scientific principles, but may contain empirical models, measured data and other simplifications, particularly where the scientific knowledge is inadequate. It is then necessary to perform extensive validation tests with field observations and to strictly limit the model to applications supported by the validation tests.

The MRT can identify several areas in which model simplifications have been made, but can not easily assess the validity of those simplifications. The MRT did examine some of these simplifications and parameters settings and had significant questions.

3.3 Documentation

Because the modeling program has been moving very rapidly and has been under pressure to produce scenario results, model documentation has not kept pace with the model development. As a result, the team had difficulty obtaining current information on model approaches and model details and the team relied heavily on discussions with the MEG, the Waterways Experiment Station (WES) staff, individual experts, and presentations and discussions in the MSC.

3.4 Model Accuracy and Consistency

To address model accuracy there must exist frequent extensive comparisons between model results and comparable field data, standards for comparison, analysis of the results and documented conclusions. Consistency similarly requires some procedure and analysis for determining model sensitivity to critical parameters. While there are some model results and observations available, analysis reports describing model accuracy and consistency, particularly in multi-dimensions, do not seem to be available. There are also many model-tuning parameters that are adjusted to obtain a better fit to measured data. The rationale for the selection of the parameters and for the parameter changes does not seem to be documented.

3.5 Review Preparation and Support

The Modeling Subcommittee did not initially appear to be prepared for this review and our requests for material were handled very slowly. Some of the reports and data that would have been useful early in the study were only available near the end of the review period.

4.0 Findings

The General and Specific Finds of the team are listed below.

4.1 General Findings

1. The Modeling Evaluation Group (MEG) was originally established as the independent technical review body. However, over time the membership and functioning of this Group has changed and it is the opinion of this Model Review Team that the MEG is not now effectively serving that purpose.
2. Because complex models require many simplifications and empirical elements, validation with measured data is essential. However, the program planning and technical planning of the modeling and monitoring efforts are not closely coordinated, making such validations difficult and questionable.
3. Documentation of the model, the validations, and results have not kept pace with the model development.
4. Publishing papers in the peer-reviewed journals is the time-tested method of obtaining technical evaluation of new scientific and engineering ideas, models and data. Very little of the Bay model has been published in those journals and apparently there has been none published recently.
5. Comparisons of modeled and measured results are based upon visual evaluations of how well the model appears to fit the data over many geographic areas and times. However, in some cases biological processes are very sensitive to the precision of the fit in narrow regimes and overall fits are not adequate.
6. There have been some notable interactions between the research community and the model development communities, but generally the interaction of the communities and the transfer of knowledge in both directions have been inadequate.

4.2 Specific Findings

The specific findings reached by the team have been grouped according to the areas for analysis in the Terms of Reference.

Question #1: Evaluate the status of the Phase IV CBP Water Quality Model and its calibration--.

1. The WQM cannot provide reliable predictions of the impact of nutrient input changes unless it accurately: a) reproduces the vertical density structure in the water column; b) accurately computes photosynthetic carbon fixation as a function of nutrient input; c) accurately computes organic carbon consumption in the water column as a function of supply, temperature, and oxygen concentration; d) accurately computes sinking of organic carbon below the pycnocline as a function of supply and; e) accurately computes the consumption of organic carbon by the benthos (including bacteria, microfauna, and macrofauna) as a function of supply, temperature, and oxygen concentration. These are minimum

requirements, but the Model Review Team had no clear summary documentation that any of these conditions were met. The small amount of information we have seen regarding vertical density structure and carbon fixation suggests that they are not. (Appendix A, B, C).

2. The circulation/hydrodynamic model does not always accurately reproduce the bottom salinity, particularly in the deep channel, which could represent an important discrepancy when biology and oxygen are considered. (See Appendix A for details.)
3. For those areas where we were shown light attenuation predictions and measurements, discrepancies where considered to be significant.
4. The Water Quality Model markedly under predicts phytoplankton photosynthetic rates, which seriously limits its credibility as a tool to quantify relationships between nutrient inputs and oxygen concentrations. (See Appendix B for details.)
5. The seasonal cycle of oxygen concentration/depletion is superficially well represented in the WQM. However much of the cycle is a simple function of water temperature. It is less clear that critical periods of biologically driven hypoxia are in fact simulated reliably.
6. The plankton food-web structure is crudely represented. This shortcoming limits the utility of the model for prediction of changes in response to nutrient reduction, variations in flow, etc. In particular, the microbial loop, phytoplankton functional groups and zooplankton community structure, including gelatinous predators, need to be better formulated and included in a revised or new model of water column ecology. (See Appendix C for details.)
7. Suspended sediment is possibly the major agent of light attenuation and nutrient transport in the Chesapeake Bay. Sediment transport is not currently well represented in the model.
8. Some of the important properties being predicted by the models have not been adequately compared with observations. In some cases, the relevant observations do not exist or were not made on appropriate time and space scales for model comparison.
9. The primary emphasis in the model has been with the state variables (e.g., chlorophyll standing crop and dissolved oxygen) and less attention has been directed to important rate variables, such as, primary production and water column oxygen consumption that really determine the state variables.
10. The benthos model, which the Modeling Subcommittee believes is not working properly, is still used interactively with the WQM.
11. The models were intentionally designed not to handle event-scale occurrences, such as, frontal passages, major storms and hurricanes. However, these events can have significant impact on biological processes and sedimentation.

Question #2: Review the linkages and coupling of model components---.

1. The Watershed Model and the Water Quality Model are generally run sequentially as one integrated model, making it difficult to determine which model is the primary contributor to observed problems.
2. The coupling of the coastal ocean to the Bay provides a very strong influence that does not appear to be modeled with sufficient detail, particularly in regard to nutrients.
3. The MRT decided that other linkages, e.g., watershed and airshed, were beyond its ability to review adequately given its expertise and the time and information available.

Question #3: Identify ways to increase the utility of the model and its products---. (See General Recommendations and Future Directions below.)

Question #4: Identify areas of the CBP model requiring additional development---.

1. Improve the coastal ocean model component by adapting one of the existing models available in the published literature.
2. Develop state-of-the-art biological models in conjunction with the monitoring community to insure that predictions and measurements can be usefully compared.
3. Update the light/primary production component of the WQM.
4. Include suspended sediments as a dynamic variable in the model.
5. Devise a method to handle event-scale processes.

5.0 General Recommendations

In the Water Quality Model the representation of several important biological processes produces results that differ dramatically from Bay measurements and current scientific understanding. It is the opinion of this team that the Water Quality Model does not currently provide information suitable for major management decisions and that use of the model for such purposes should be suspended. Some recommended steps to address these problems are listed below. The stated issues and the recommendations are paired below.

1. The modeling program appears to lack a healthy culture of openness, access, and scientific skepticism. We saw little evidence that MEG now functions as an objective quality control mechanism. This is not to say that it has not served such a role at times in the past, but it was not evident to us at this time.

   Review the role of MEG as an objective quality review mechanism and make appropriate changes; for example, consider term limits and a different management reporting structure.

2. The Modeling Subcommittee and the Monitoring Subcommittee do not appear to function cooperatively, which apparently works to the disadvantage of both subcommittees. It certainly limits the ability to validate model results.

Redesign and re-implement the Monitoring and Model programs to function as coordinated, mutually supporting elements of the overall Bay Program.

3. The last major effort to document the model occurred in 1994, with only minor additions since then.

   Model documentation and results need to be made available to the scientific and educational community as well as management agencies. Some of the model results have been put on an Internet web site, however, some of the team members tried to access the data and found it difficult to use.

   A documentation library of the model, validation procedures, analyses, and results should be maintained so that future reviews will have a written database of material to review.

4. Heavy demands have been put on the modeling staff to produce a vast array of scenarios before the credibility of the model could be established and documented.

   Model development, documentation, validation and projections should be published in the peer-reviewed scientific literature to provide a basis for accuracy and accountability. This is the only way to insure that the Model and its elements are formulated according to the best available information and that the results are in agreement with peer knowledge.

5. The techniques used for comparing model predictions and measured data appear to be based upon subjective judgement without objective means of evaluation or sensitivity analyses.

   Greater emphasis should be directed to objective analysis and sensitivity studies.

6. While there has been ongoing interaction between the MSC and the research community, there have not been many joint or cooperative efforts and much of the current university-based research is not reflected in the model. This is a significant problem since the model is pushing knowledge in several fundamental areas.

6.0 Future Directions

Several of the observations led to suggestions that have longer term or more profound implications[1]. Those were separated out and are listed here.

1. The current trend in atmospheric, physical oceanographic and ecological models is to use data assimilative techniques that allow inclusion of data to drive boundary conditions and allow components of the model to be replaced with observed data. This is particularly valuable where the scientific knowledge of specific processes is lacking. The MSC should be investigating these models as future replacements for or refinements to the existing model.
2. Consider major changes to the structure of the hydrodynamic model along the lines of finite element techniques that have become the preferred approach in the university-based research community. If the current model is well documented and easily available it can continued to be used for years by the academic community and other stakeholders.
3. Improve interaction with the research community (staff and students) so the research will be better coupled into the model and so the academic community can better benefit from the knowledge gained from the model. Graduate thesis involving both model and monitoring results could be encouraged.

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* As a result of the early draft versions of this report, the Corps of Engineers reviewed and modified the representation of respiration in the Water Quality Model. Since the new results were available before the report went to press, this appendix has been revised to reflect the newer model results. While still not in agreement with measured data, the revised model does produce noticeably better results.

Appendix A-Simulated Salinity Accuracy

The accuracy of the circulation model is an important issue for this review because the circulation determines to a large extent the distribution and concentration of the biological and water quality state variables. Salinity is the variable used for assessing the accuracy of the circulation model. Salinity is also potentially an input to the biological models through rate functions that describe physiological responses to changing salinity environments.

The results of two types of analyses that have been used to assess the accuracy of the salinity fields produced by the Chesapeake Bay circulation model have been made available for this review. The first consists comparisons between simulated salinity distributions and observed salinities that have been averaged over a season (e.g. March to May) and also averaged over multiple years (e.g., 1985-1988). The second is comparisons between salinity distributions from specific simulations and measurements from specific times and locations. Ten-day averages were used for these comparisons.

The long-term averages (Figure 1) show that the simulated salinity distributions at selected sites along the main stem of the Bay generally fall within the variance of the observed salinity measurements and that trends, such as the up-bay decrease in salinity, are captured in the simulations. However, this type of comparison is not a rigorous test of the model capability or skill. Averaging the observed salinity over season and then over years causes interannual variability in the salinity measurements to appear as variance in the data. The result is increased variance in the observations due to such things as year-to-year variability in the timing of fresh water events. Similarly, partitioning the observed and simulated salinity by season assumes year-to-year repeatability of the seasonal signal in salinity. Again any interannual variations in this will show up as added variance in the measurements. The fact that these comparisons show simulated salinities that fall within the range of the measurements is not surprising given the lack of robustness of the approach.

However, even with with long-time averaging, comparisons of observed and simulated salinity show that the simulated bottom salinities along the main stem of the Bay consistently overestimate the observed values. The overestimation of bottom salinity is clearly demonstrated in the averaged vertical profile comparisons for selected sites along the mainstem of the Bay (Figure 2). This suggests a problem with the salinity boundary condition at the Bay entrance. Plotting the model-derived salinity versus the observed salinity would provide a estimate of the scatter as well as indicate whether or not there is a consistent bias in the simulated salinity distributions. This has not been done as part of this review, but should be done at some point.

Comparisons between simulated and observed salinities based on ten-day averages at selected sites in the bay (Figure 3) show that modeled values capture low frequency trends, such as the seasonal cycle in salinity.

Higher frequency events or extremes are not captured in the simulations. These comparisons also show overestimation of the bottom salinity. This overestimation is as much as 7-10 ppt at site CB7.3, which is near the Bay mouth. Bottom salinity at site CB2.2 in the northern Bay is also consistently overestimated. Bottom salinity at other sites, such as EE3.2 in the middle portion of the Bay is consistently underestimated.

Simulations of surface salinity show a better match with observations, with simulated salinity values being with 1-3 ppt of observed values. However, high frequency variations or extreme events in surface salinity are not captured in the simulations.

The following sections discuss the potential effects of inaccuracies in the simulated salinity, especially at the bottom, on circulation and on physiological responses by benthic organisms. The effect of salinity on benthic organisms is not now included in the Chesapeake Bay biological model. However, this could possibly be included in future versions of the model.

A. Circulation Effects

The alongstem bottom salinity gradient in Chesapeake Bay, and any other estuary, is an integral part of the processes that determine the estuarine overturning rate that is associated with the gravitational circulation. The top-to-bottom salinity gradient determines the vertical stratification in the estuary. The simulated bottom salinities from the Chesapeake Bay circulation model result in the alongstem and vertical salinity gradient being too strong, relative to what is expected from observations.

The effect of incorrect simulation of these gradients is to diminish the amount of vertical mixing that occurs in the Bay. The net effect is that oceanic water, with its higher salinity, intrudes further into the Bay, making the bottom waters more oceanic in character. The lack of mixing allows the salinity excess to remain intact rather than being eroded and diluted by mixing with the fresher surface waters.

The effect of the reduced mixing is to shift bottom isohalines, corresponding to higher salinities, further into Chesapeake Bay. This in effect changes the overall circulation structure of the Bay. Another effect of intrusion of high salinity into the Bay is to allow, in the simulations, the existence of high salinity organisms in areas of the Bay where they may not normally occur. This has considerable implications for inclusion of a benthic model component.

Another implication of the overestimate of the alongstem bottom salinity gradient is that the offshore boundary condition used to force the circulation model is incorrect. The continued mis-match in the lower Bay after multiple years of simulation strongly suggests a problem with the boundary condition at the Bay mouth. If the model is constantly forced incorrectly, then there not any reason to expect accurate simulated circulation distributions.

B. Biological Effects

The effect of salinity on most marine organisms is usually confined to the extrema of the range of salinity that the organism can tolerate. For benthic organisms in mid-latitude estuaries, the upper range at which salinity has an effect, usually above 35 ppt, is not normally encountered. It is salinities at the lower end of the range, usually below 15 ppt, that have a regulating effect on physiological rate processes. Significant decreases in physiological rate processes, such as filtration and respiration rate, occur in the range of 5 to 3 ppt.

Given the above, the overestimate of bottom salinity in the mainstem of the Bay would seem to be inconsequential for benthic organisms because the observed salinities are generally above 15 ppt. However, in the upper Bay and in the Bay tributaries, this is not the case. Observed salinities in these regions do fall below 15 ppt, and at some locations, such as CB2.2 salinities are always below 15 ppt. These are regions where significant benthic populations of bivalves (e.g. oysters) do occur. Salinity-dependent filtration and respiration rates for benthic bivalves are given to illustrate the potential effect of simulated bottom salinity that is too high or too low.

a. Bottom Salinity Effects on Filtration Rate

The filtration rate relationship is based on the relationship given by Doering and Oviatt (1986) which is adapted to bivalves using the biomass-length relationship given by Hibbert (1977). These relationships are of the form:

filtration rate: $FR = K^{0.96}\ T^{0.95}/2.95$ (1)

biomass-length: $K = W^{0.317}\ 10^{0.669}$ (2)

where filtration rate (FR) is in ml filtered $ind^{-1}\ min^{-1}$, and is function of temperature (T, C) and animal weight (W, g AFDW).

Filtration rate decreases below 7.5 ppt and ceases at 3.5 ppt (Loosanoff 1953). The decrease in salinity between 7.5 and 3.5 ppt is given by:

$$FR = FR(S - 3.5)/4.0 \qquad (3)$$

where S is salinity.

For a one gram ash free dry weight animal at 20 C and salinities above 7.5 ppt, equation (1) gives a filtration rate of 25.6 ml filtered/individual/min. This value provides a reference rate for comparison with the filtration rates obtained at salinities below 7.5 ppt. Simulated bottom salinities at site CB2.2 for which there are corresponding observed salinities were used with equations 1-3 to estimate the effect of the difference in the two on filtration rate (Table 1). For the low salinity environments, the simulated bottom salinities gave filtration rates that were usually 87% to 100% of the reference rate. In contrast, the observed salinities gave filtration that were either zero or significantly reduced relative to the reference rate. The disturbing aspect of these comparisons is that the simulated salinities allow significant filtration by benthic bivalves at times when observed salinities indicate that filtration should be suppressed or cut off. For other sites, such as the Potomac River, the simulated bottom salinities underestimate observed. The difference in the two is sufficient to cut off benthic filtration when it should actually be operating at 87.5% of the reference rate. The time series of simulated bottom salinities at CB2.2 indicates that filtration would occur at this site essentially all of the year. The observed bottom salinities, however, suggest that filtration by benthic communities would be greatly suppressed or nonexistent for large parts of the year. The overestimation of benthic filtration is potentially a significant effect for the biological distributions produced by the Bay model.

Table 1. Effect of bottom salinity on filtration rate. Filtration rate is given in ml filtered/individual/minute. The filtration rate calculated using the observed salinity value is designated by FR-O: that calculated using the simulated salinity is designated by FR-S.

Site	Obs. Salinity (ppt)	Sim. Salinity (ppt)	FR-O	FR-S	% of 20 C FR	
					FR-O	FR-S
CB22	3	7	0.0	22.4	0	87.5
CB22	7	12	22.4	25.6	87.5	100.
CB22	5	11	9.6	25.6	37.5	100.
CB22	0	5	0.0	9.6	0	37.5
Potomac River	7	2.5	22.4	0.0	87.5	0
Pax River	15	17	25.6	25.6	--	--

b. Bottom Salinity Effects on Respiration Rate

Respiration rate as a function of temperature and bivalve weight can be calculated using the relationship given by Dame (1972) of the form:

$$R = (69.7 + 12.6\ T)\ W^{-0.74} \qquad (4)$$

Shumway and Koehn (1982) show that salinity effects on respiration differ above and below 20 C and that these effects can be expressed as:

$$r = 0.007\ T + 2.099 \quad \text{for } T < 20\ C$$

$$r = 0.0915\ T + 1.324 \quad \text{for } T > 20\ C$$

where r is the ratio of the respiration rate at 10 ppt to that at 20 ppt. The respiration rate of benthic animals tends to increase with decreasing salinity because of the stress induced by the low values. The effect of salinity on bivalve respiration increases between 15 and 10 ppt and remains at a constant maximum effect below 10 ppt. This effect is expressed as:

$$RS = R \qquad \text{for } S > 15 \text{ ppt}$$

$$RS = R\,(1 + (r - 1/5)(15 - S)) \quad \text{for } 10 \text{ ppt} < S < 15 \text{ ppt}$$

$$RS = Rr \qquad \text{for } S < 10 \text{ ppt}$$

For a one gram ash free dry weight animal at 20 C and salinities above 15 ppt, equation (4) gives a respiration rate of 321.7 ul O_2 consumed/hr/g dry weight. This value provides a reference rate for comparison with the respiration rates obtained at salinities below 15 ppt.

The primary effect of bottom salinity on benthic respiration is at sites where the salinity ranges between 10 and 15 ppt. At the CB2.2 site, the projected benthic respiration rate is lower than what would is expected from the observed salinities (Table 2). The overestimated salinity dampens the respiration response. The effect of this is that the local benthic community has a higher net production than allowed by actual environmental conditions. In regions where the simulated salinity is underestimated (Table 2) the local benthic production is underestimated.

Table 2. Effect of bottom salinity on respiration rate.

Site	Obs. Salinity (ppt)	Sim. Salinity (ppt)	R-O	R-S	% of 20 C R R-O	% of 20 C R R-S
CB22	7	12	1,012.	735.	68.2	56.3
CB22	5	11	1,012.	873.	68.2	63.2
Pax River	15	17	321.	321.	--	--
Pax River	14	8	459.	1,012.	30.1	68.2

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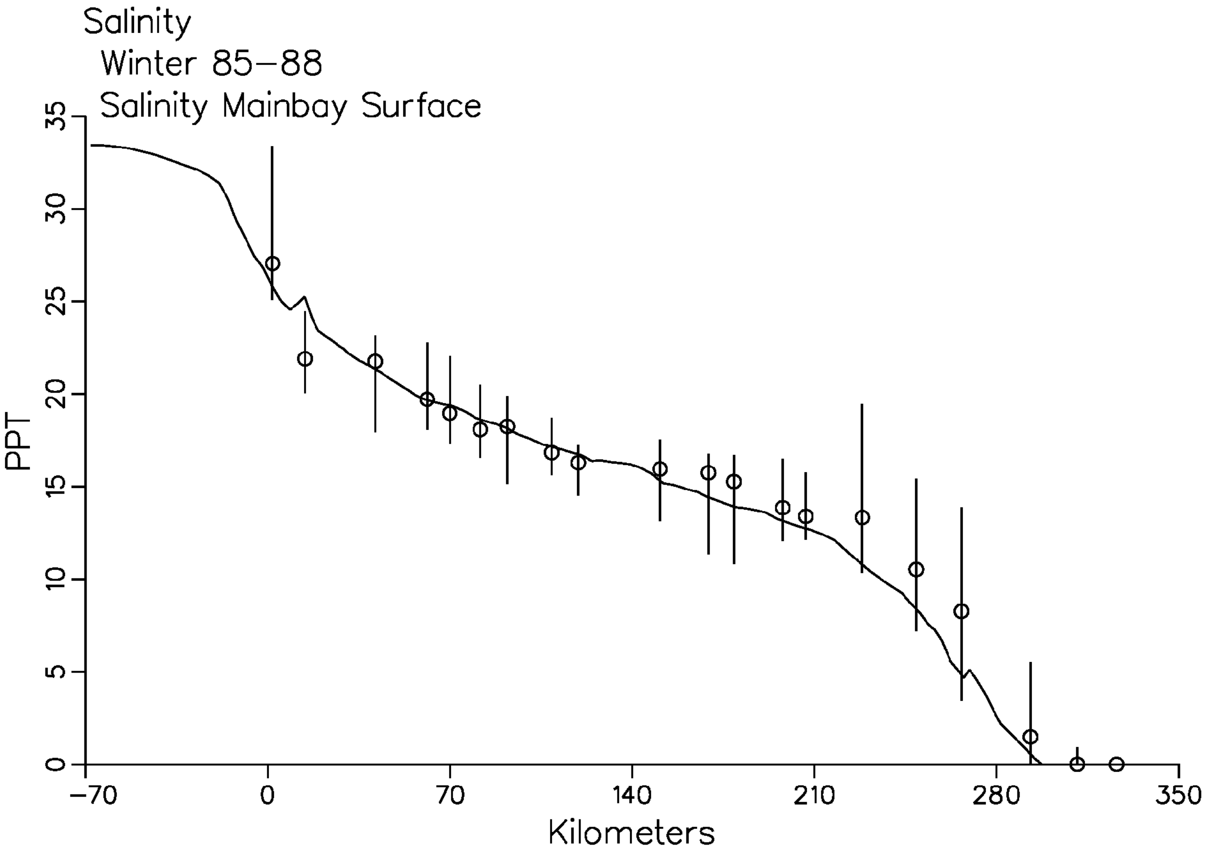
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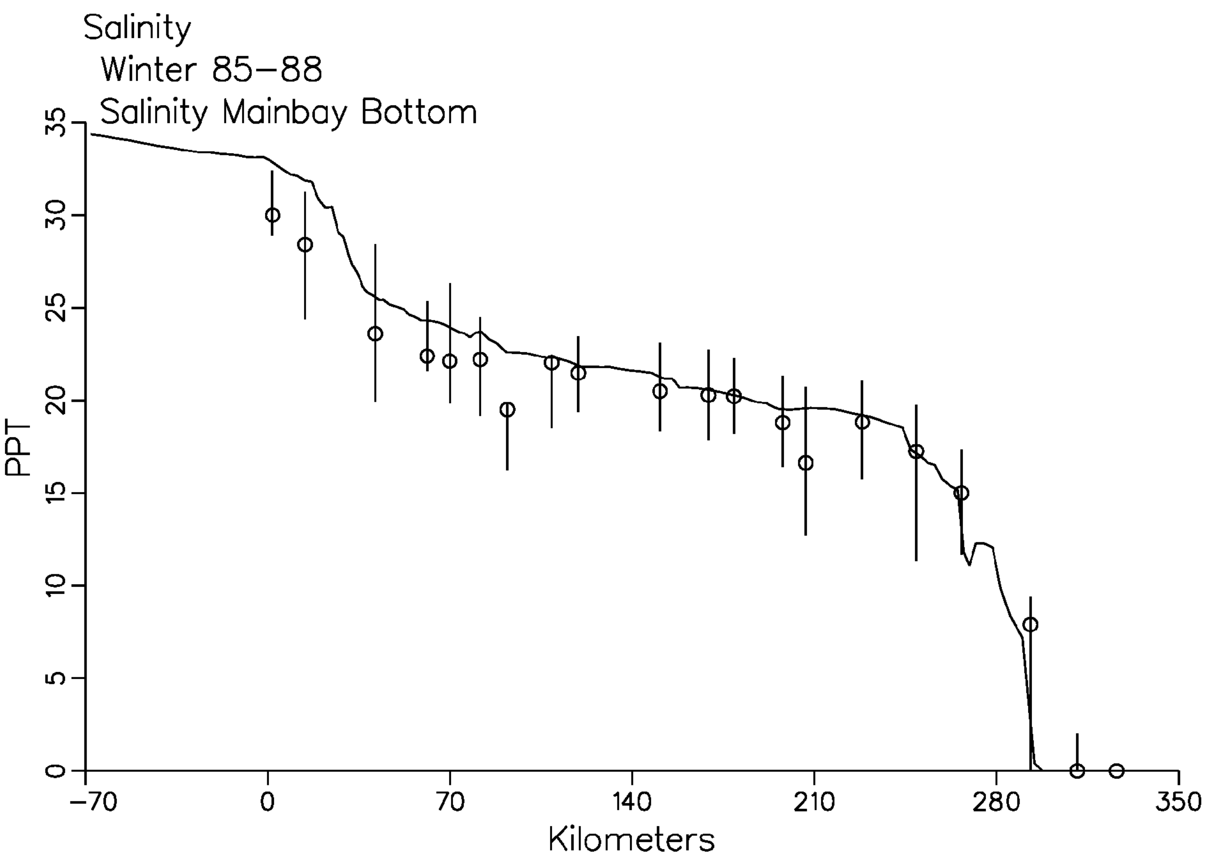
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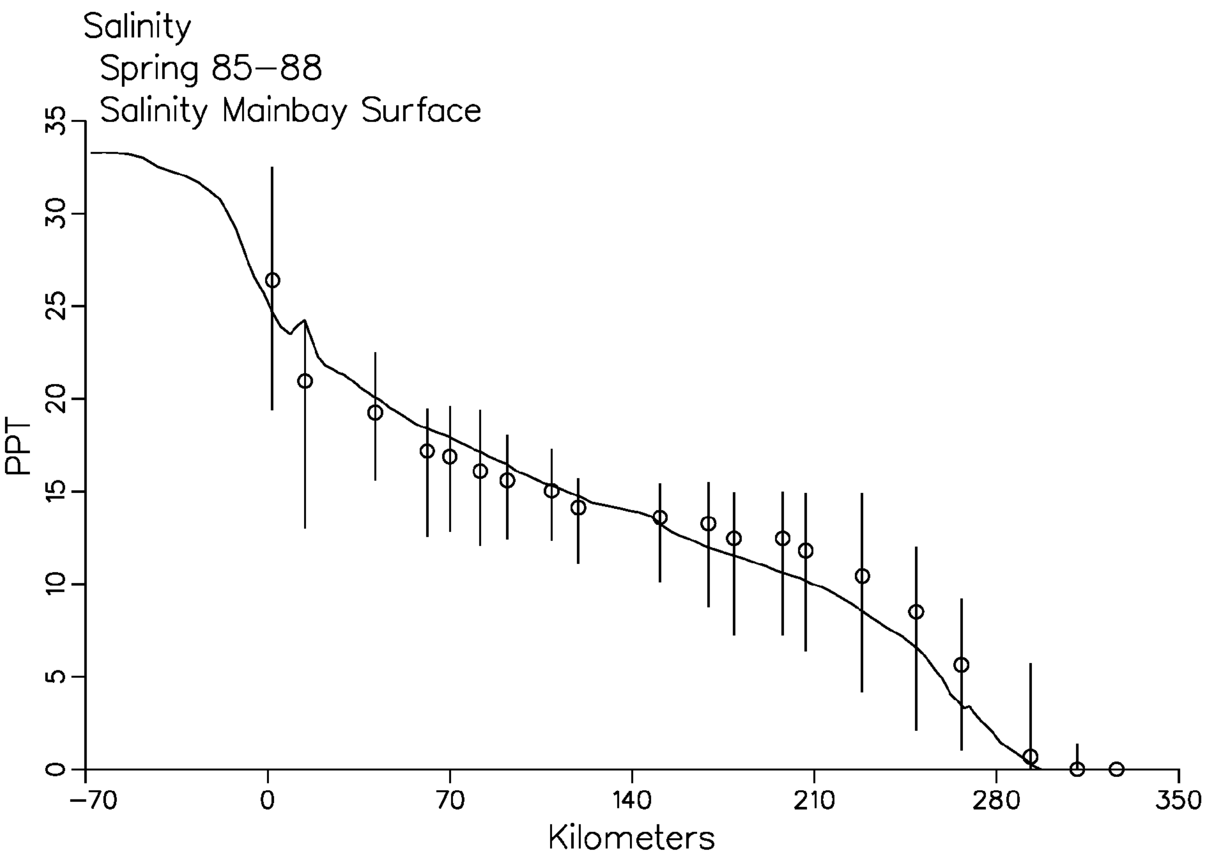
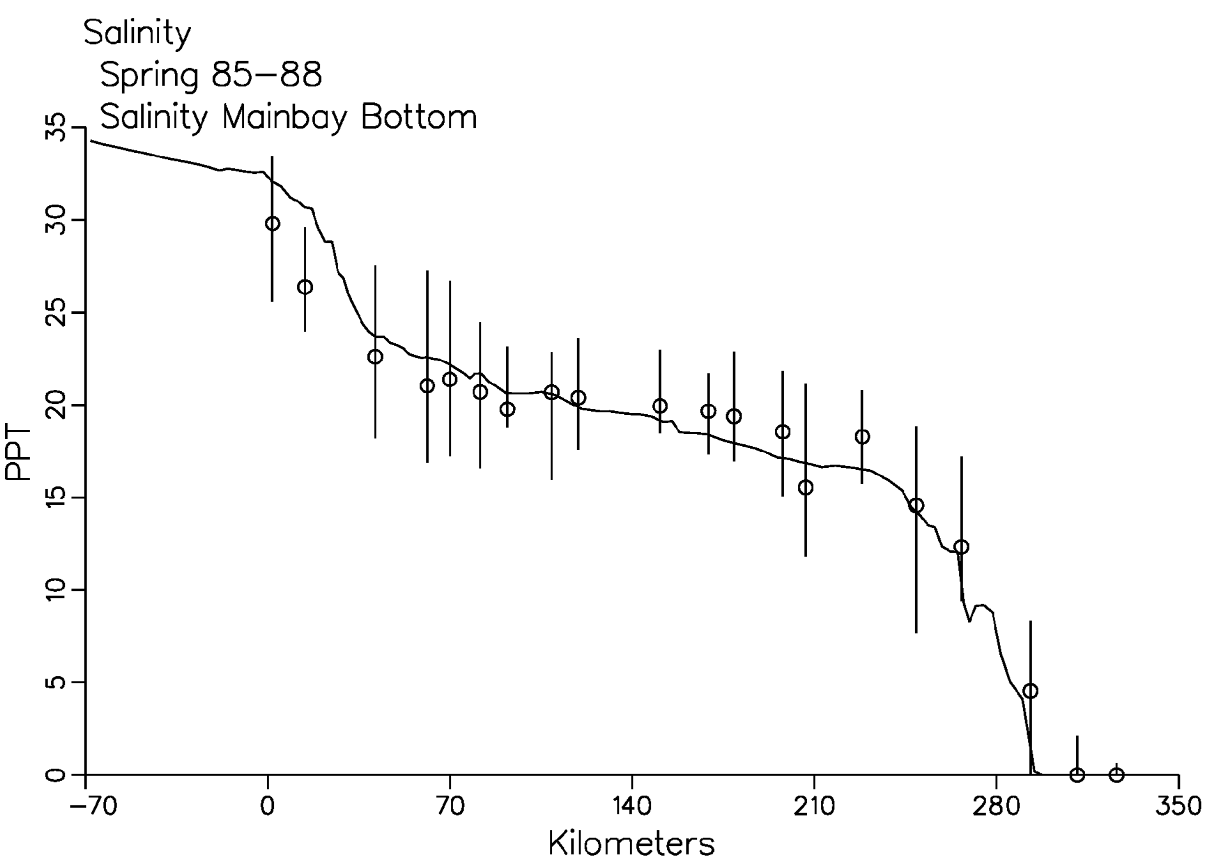
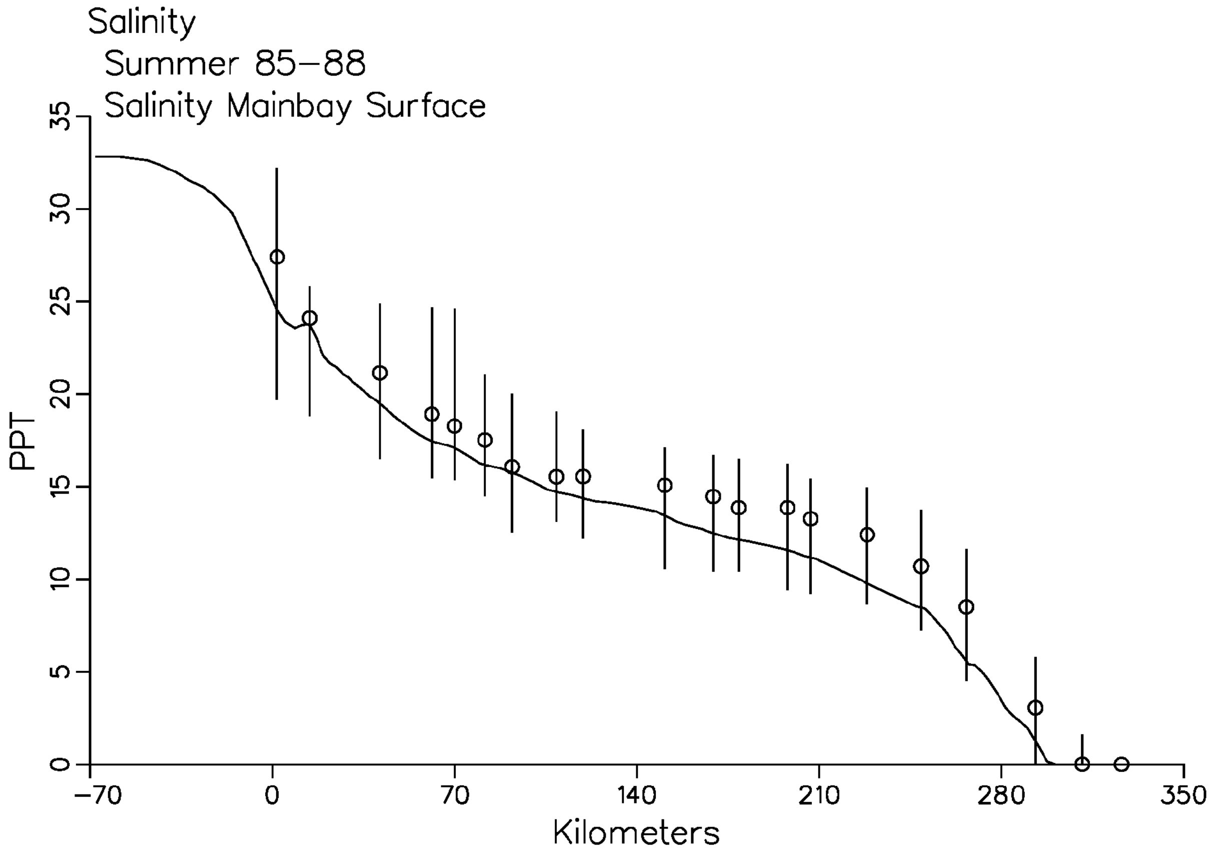
MAINSTEM BAY, (SALINITY MEDIANS) 9/7/99



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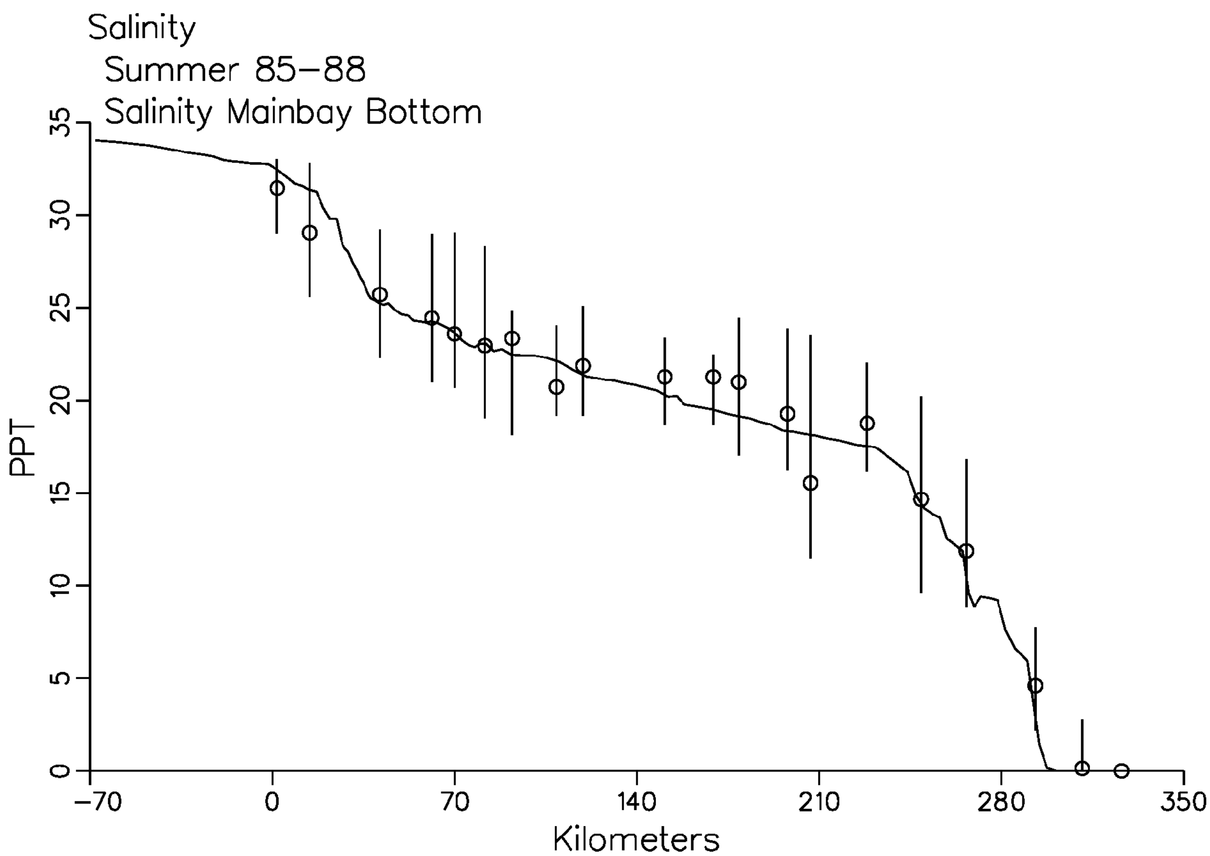
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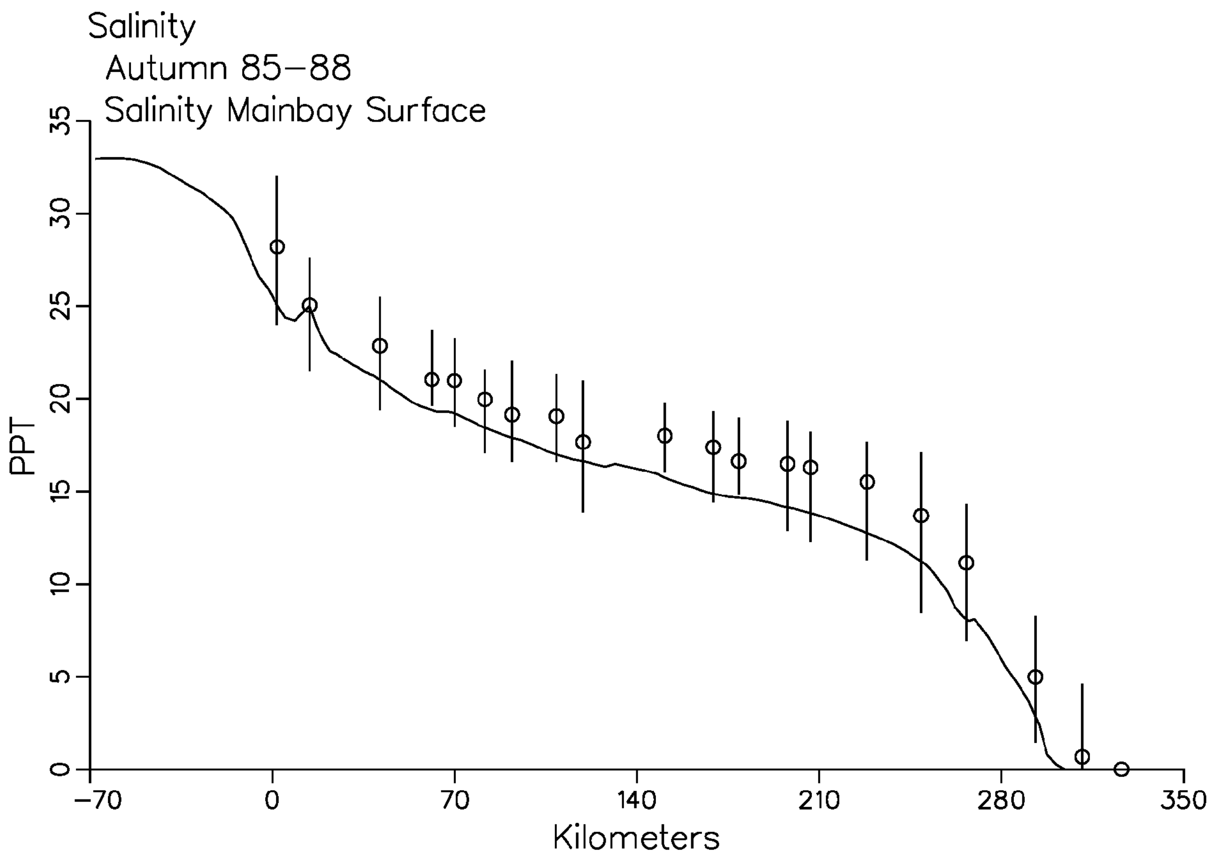
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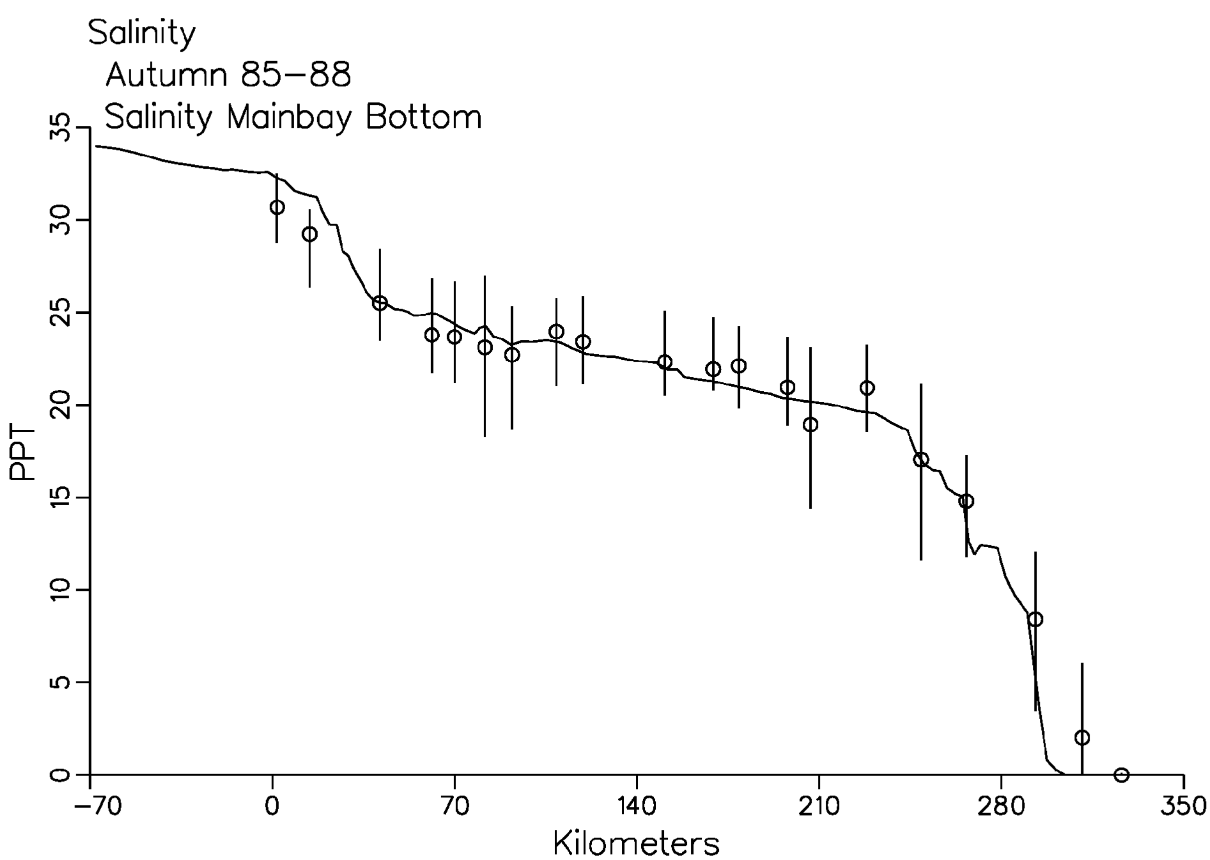
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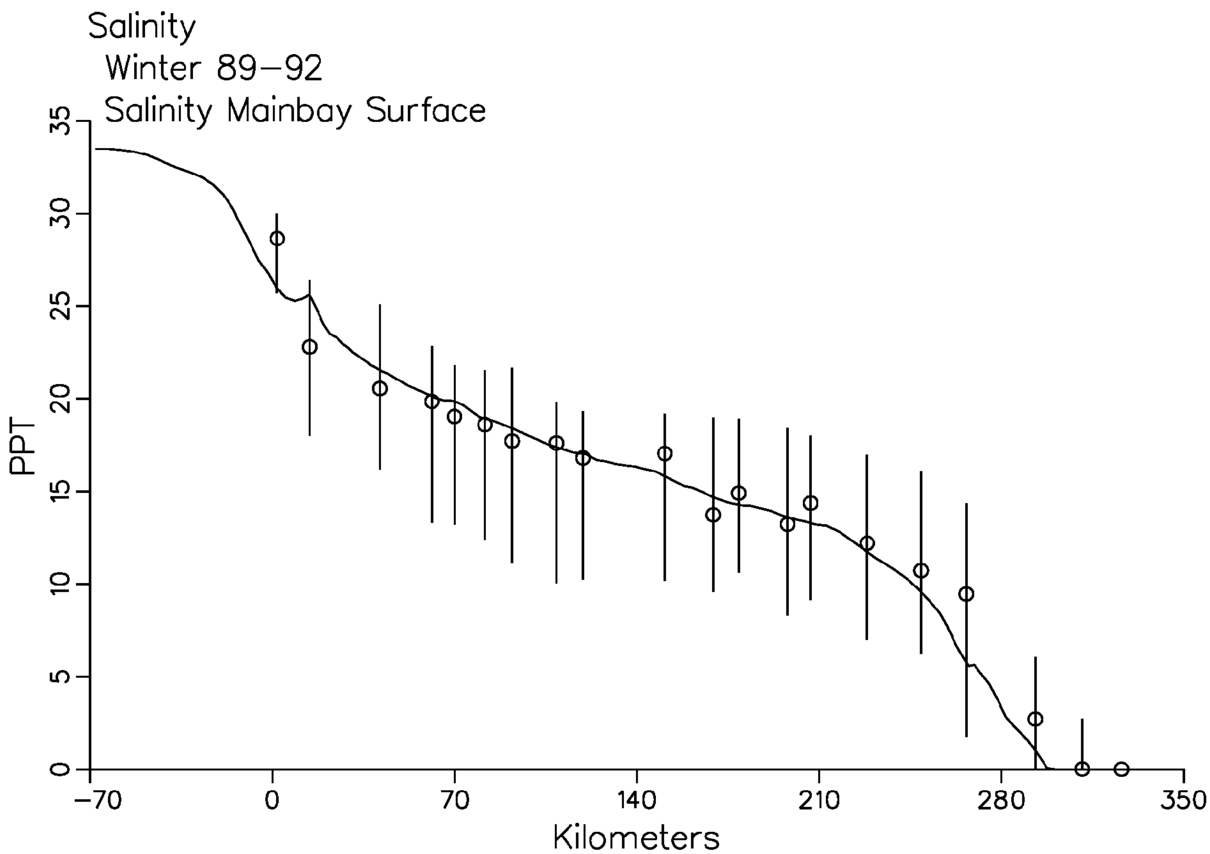
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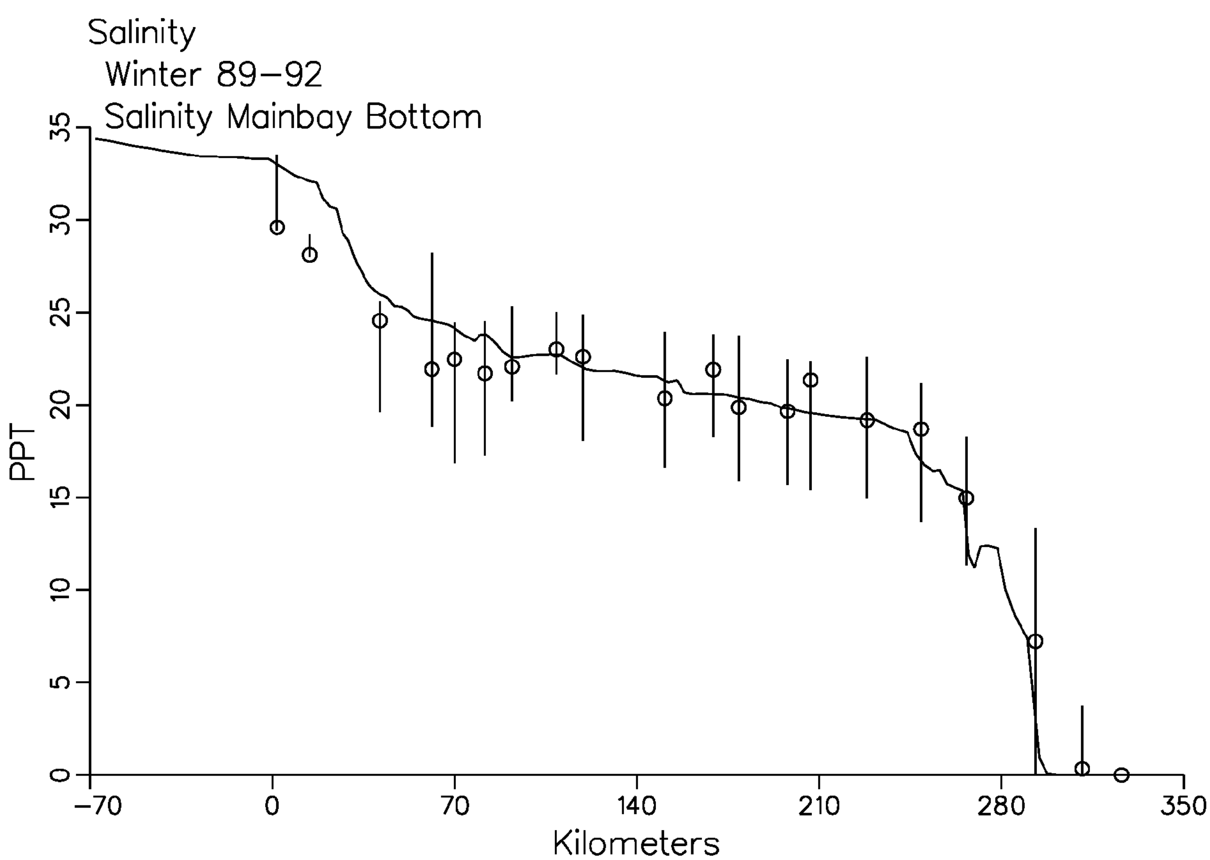
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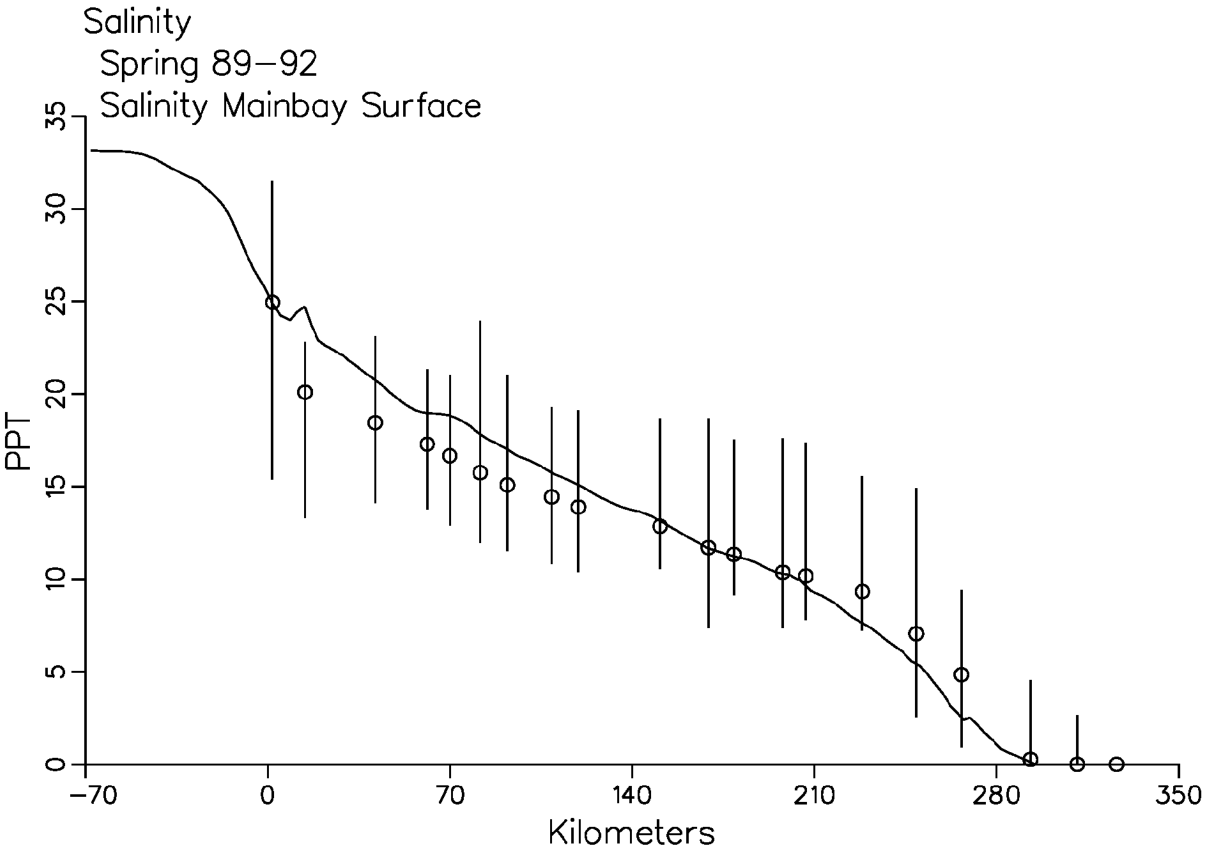
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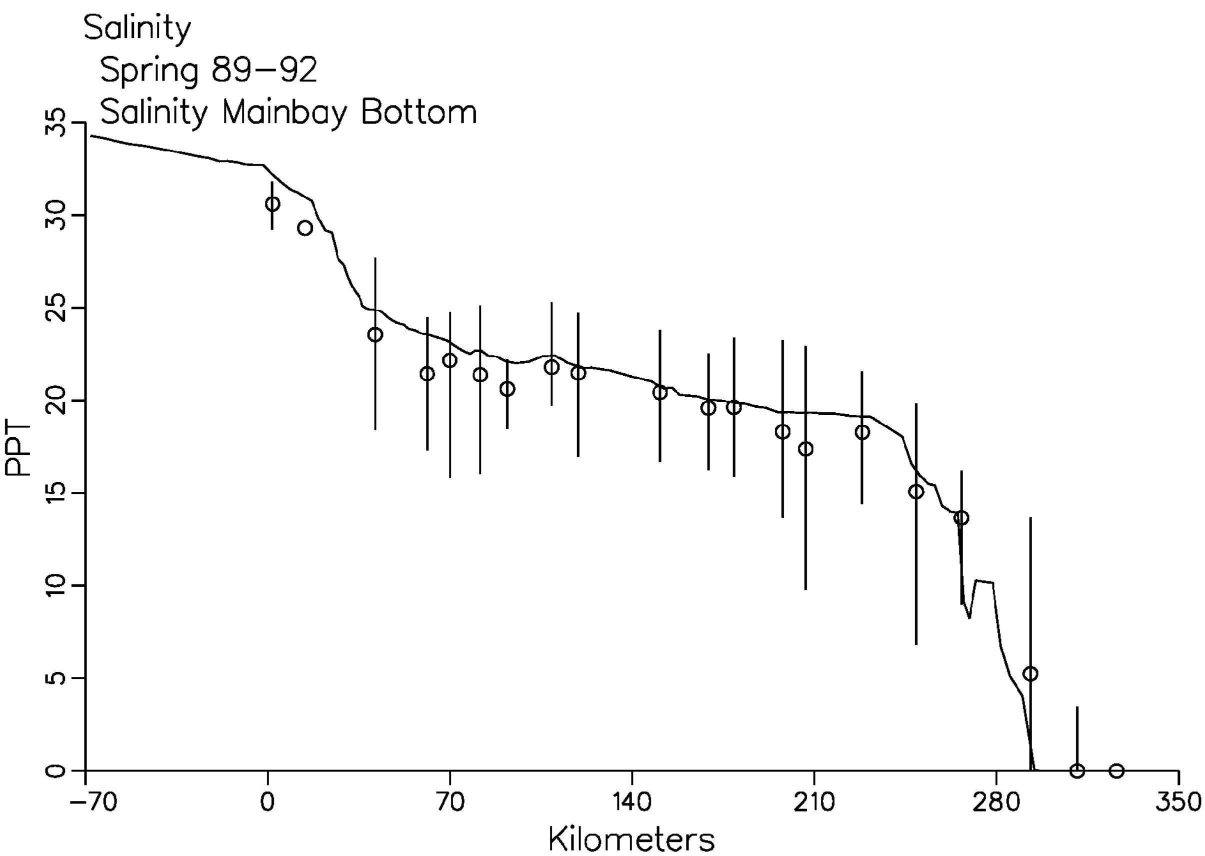
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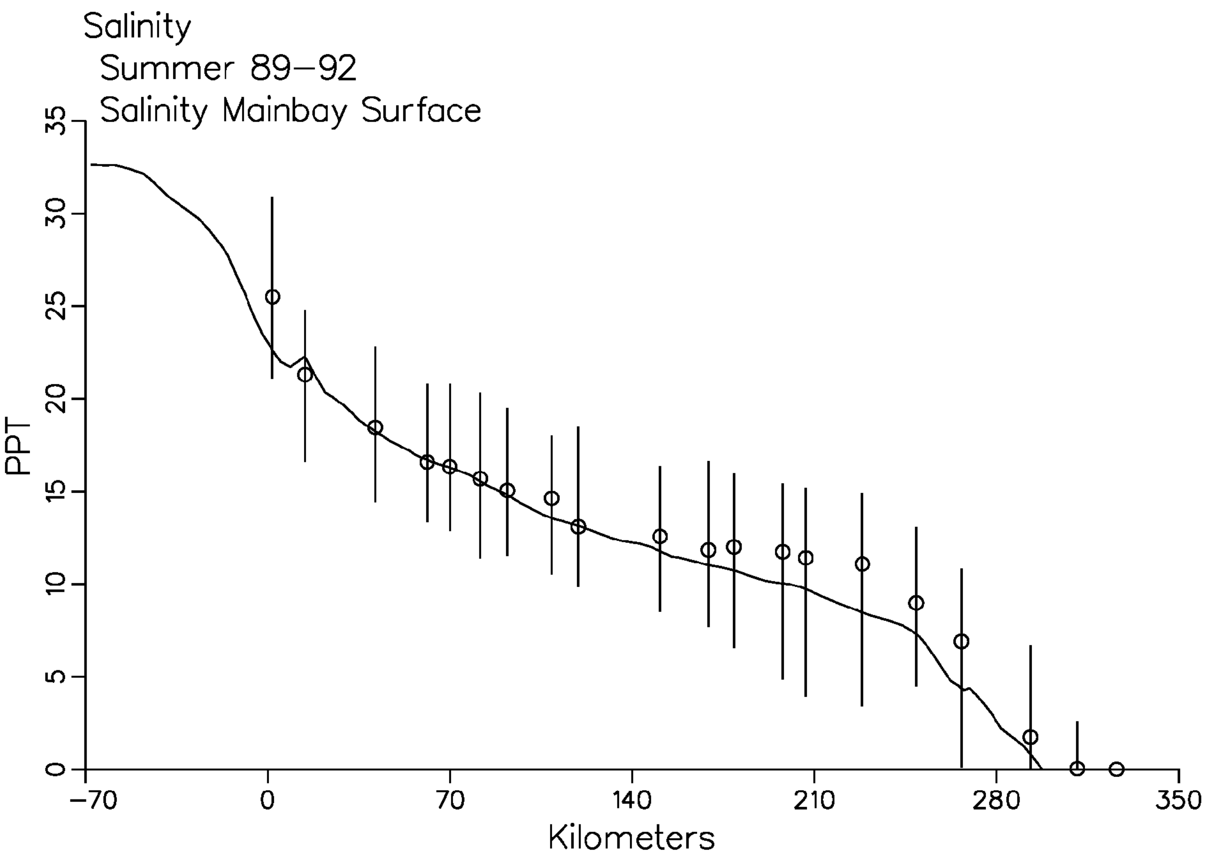

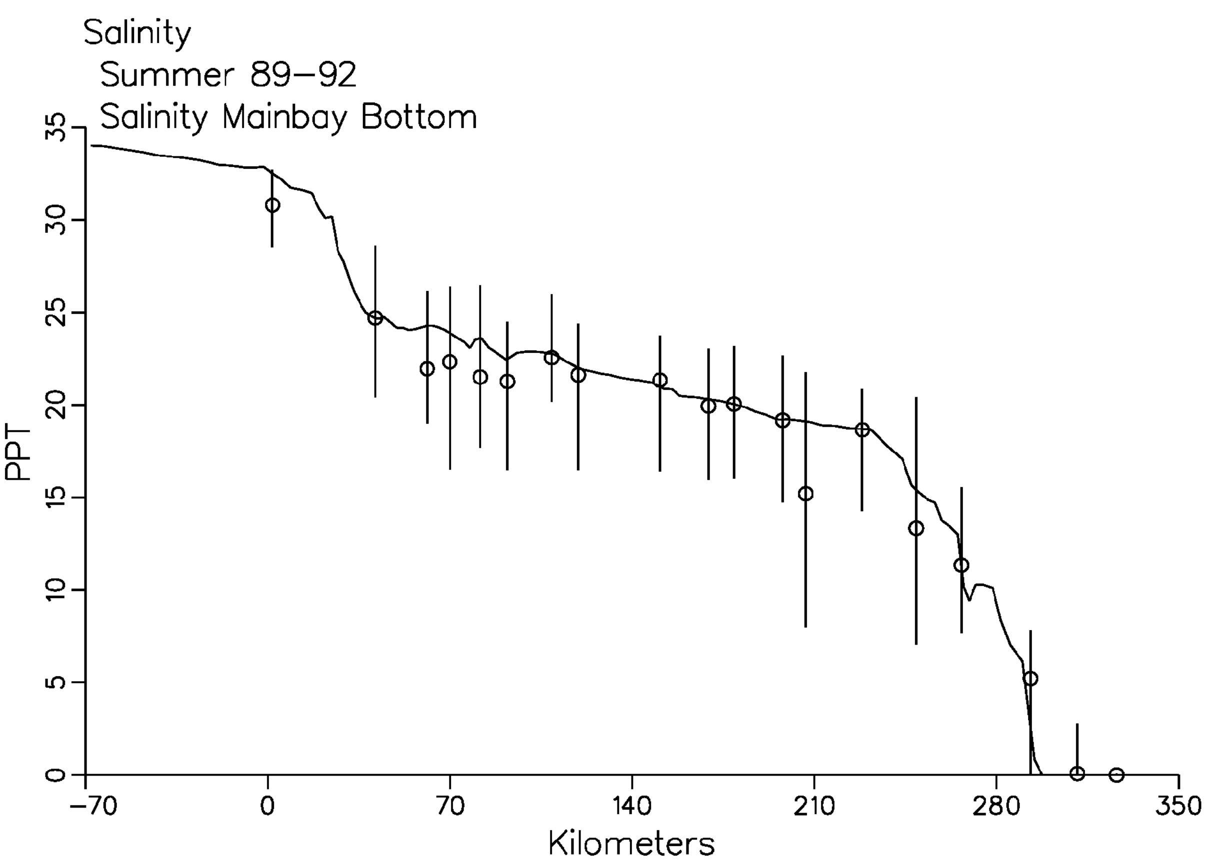

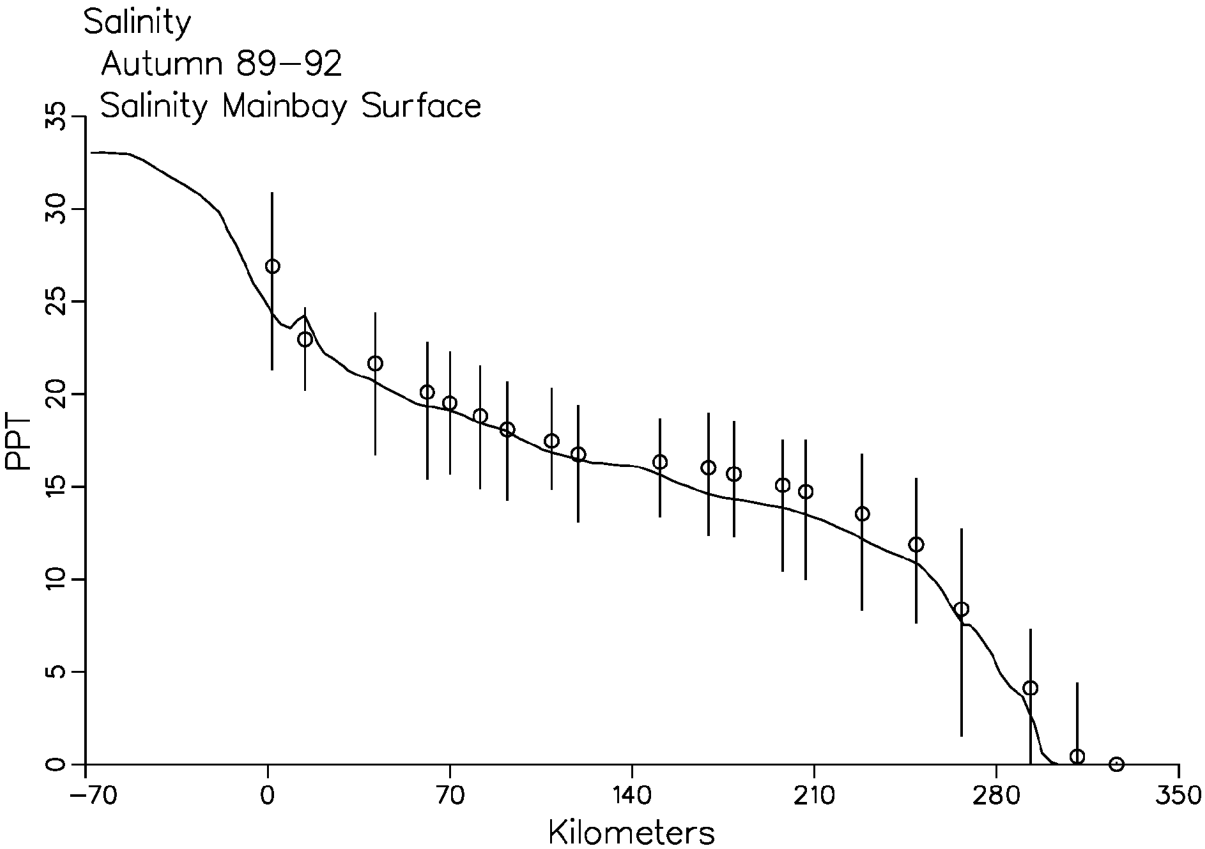
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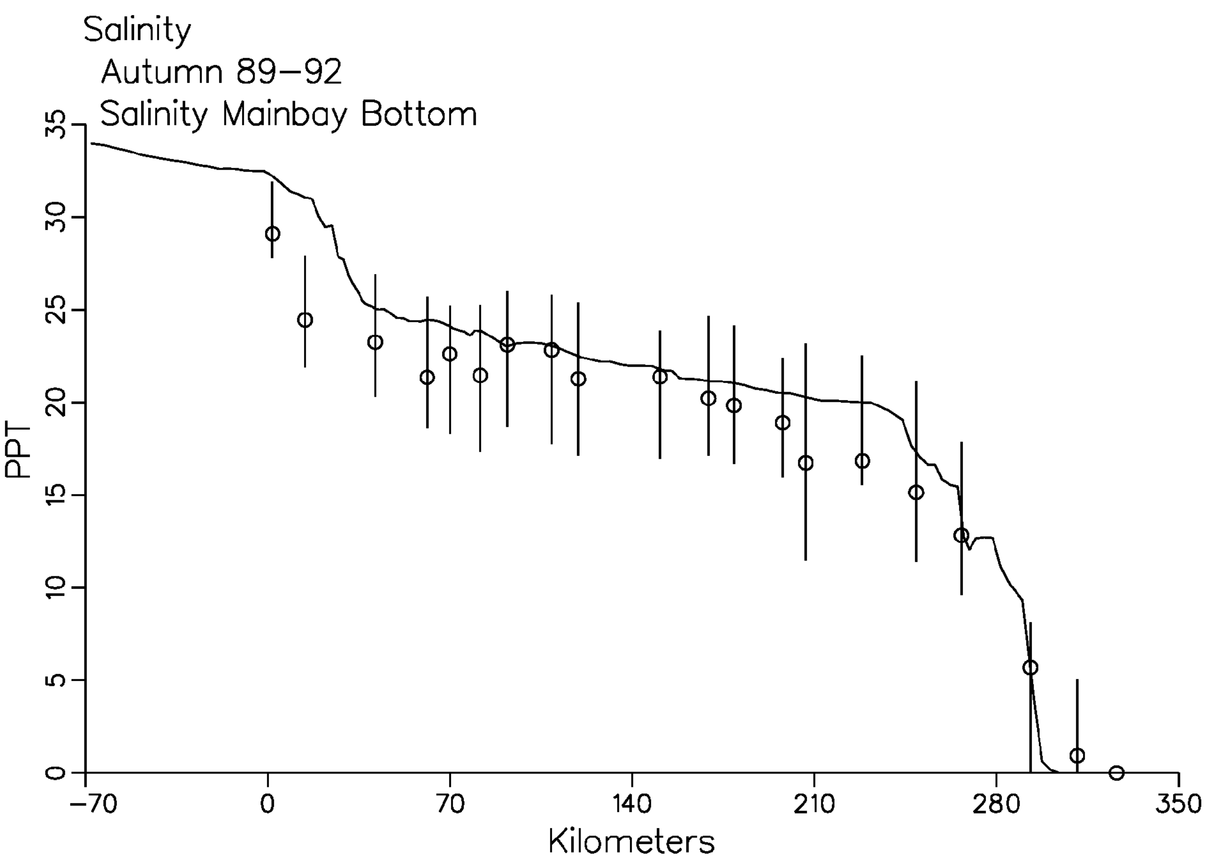
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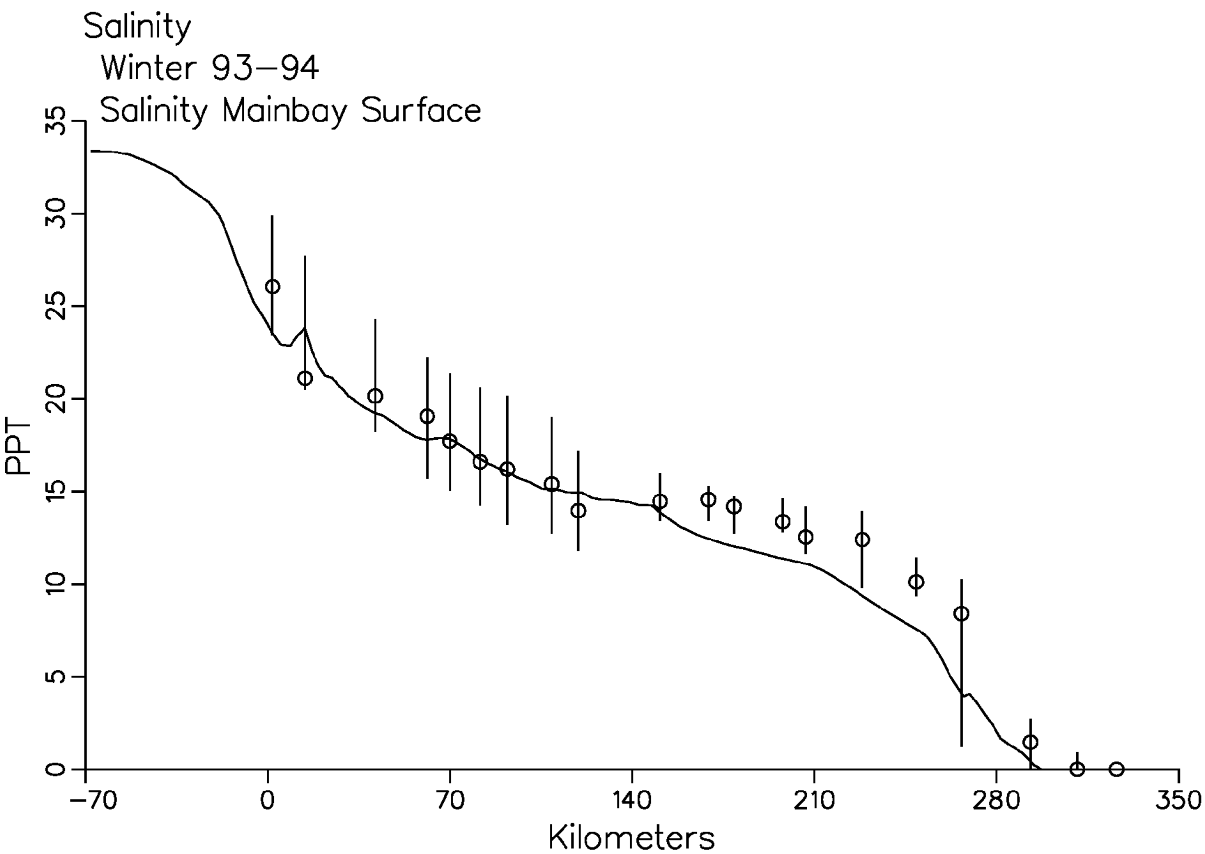
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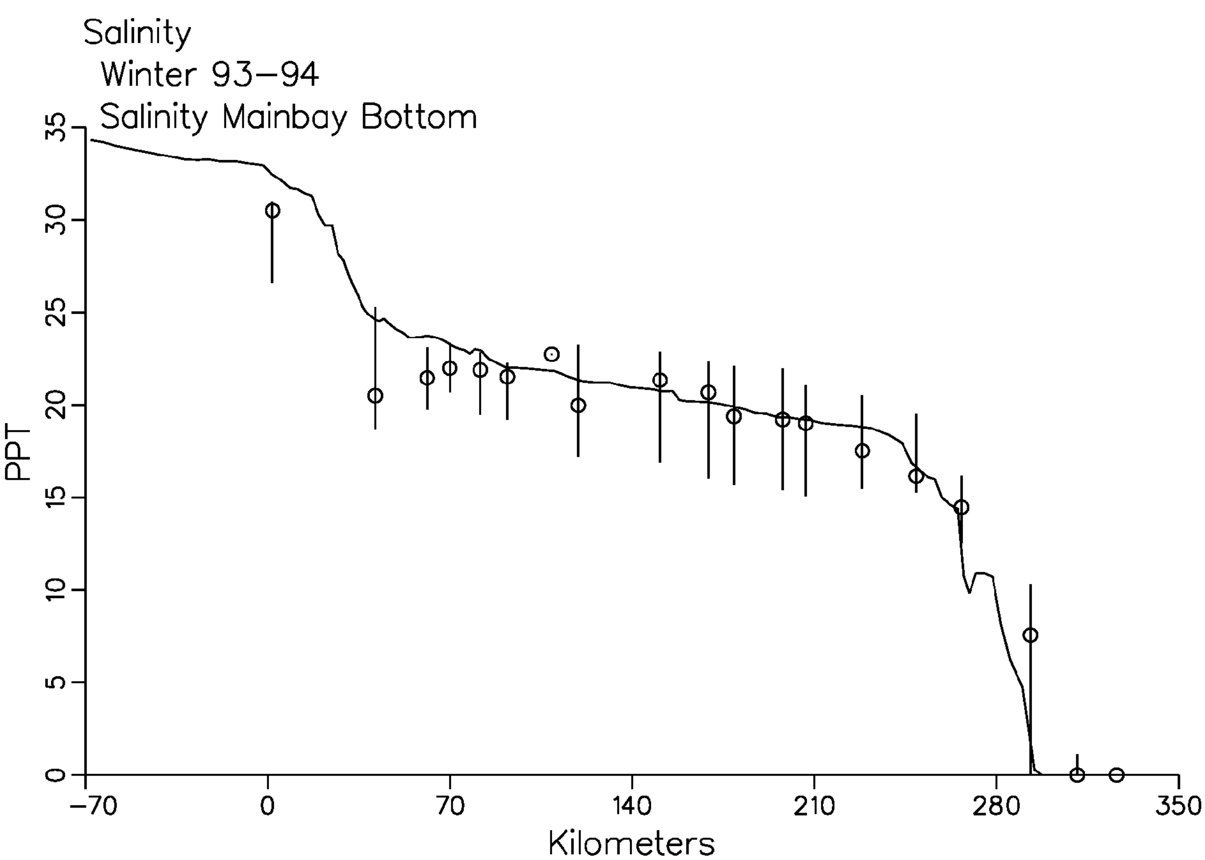
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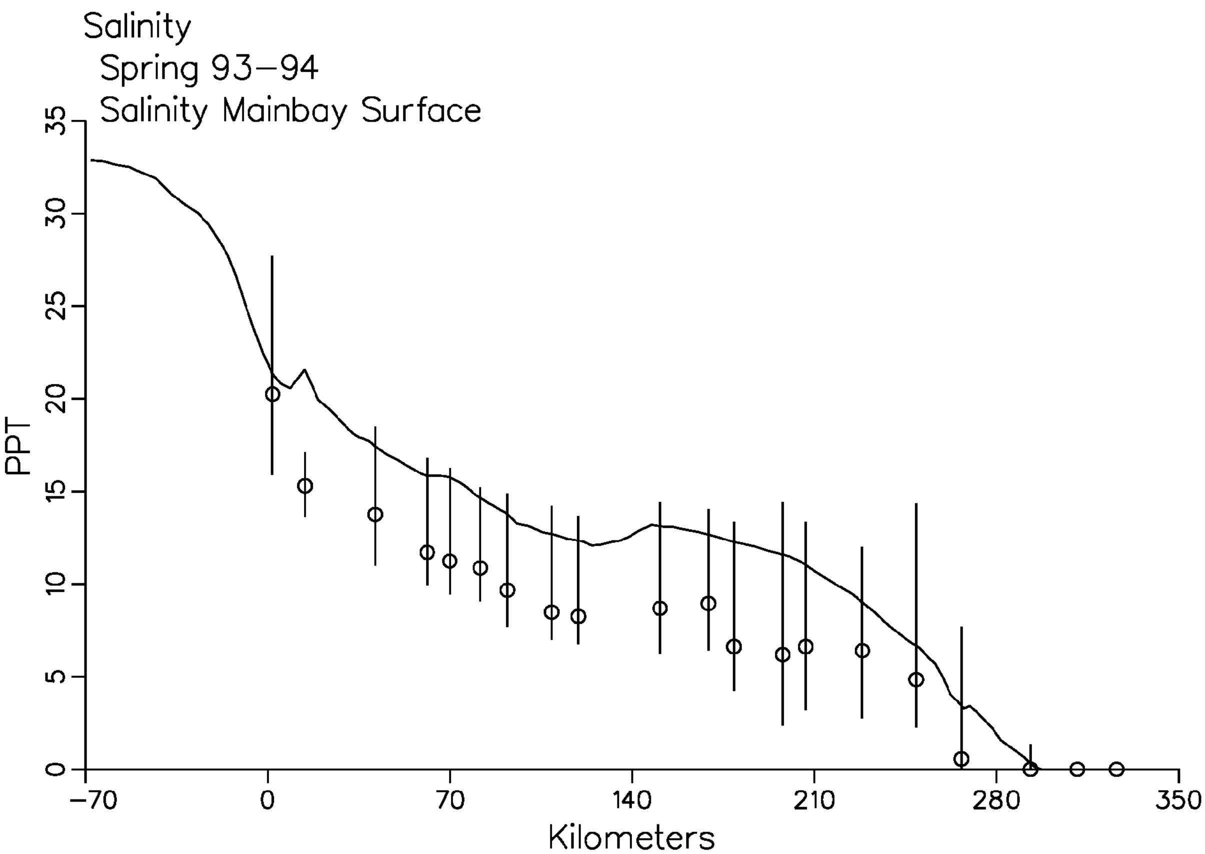

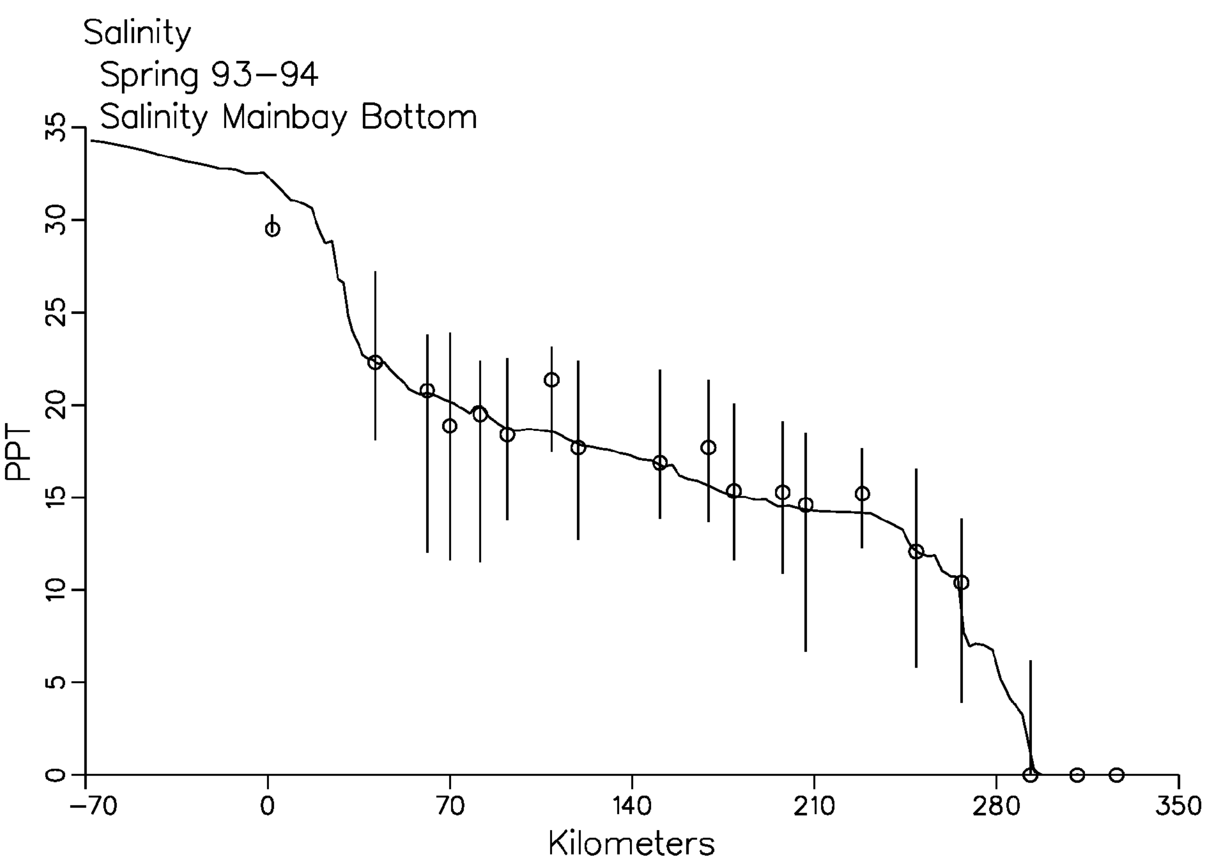

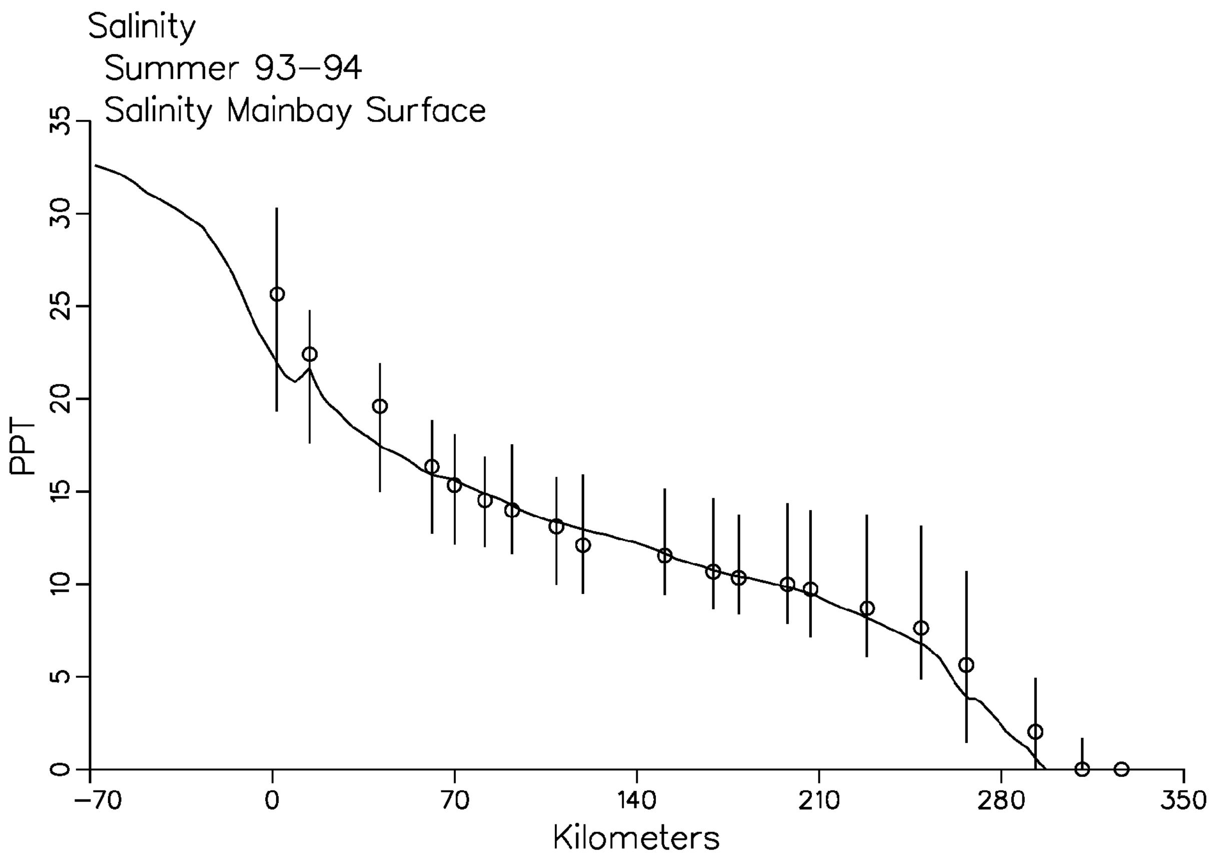
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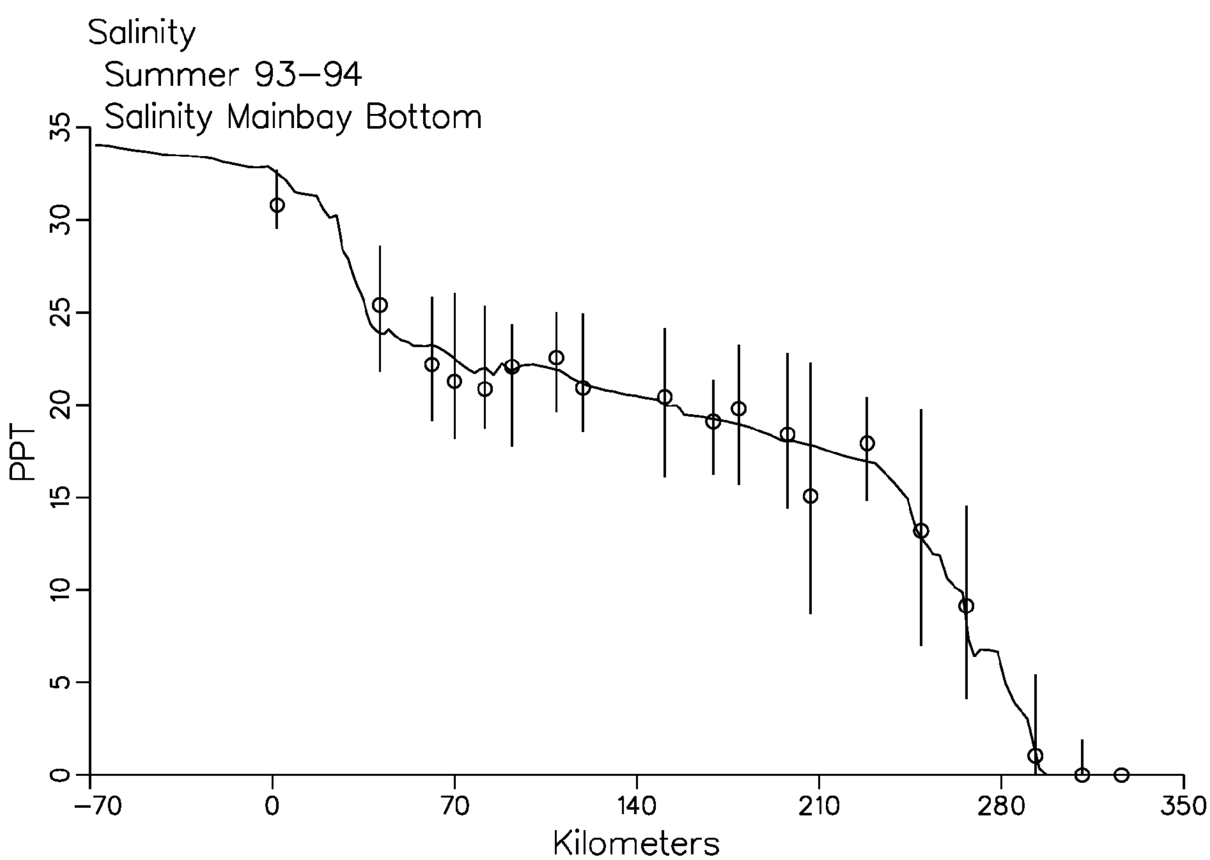
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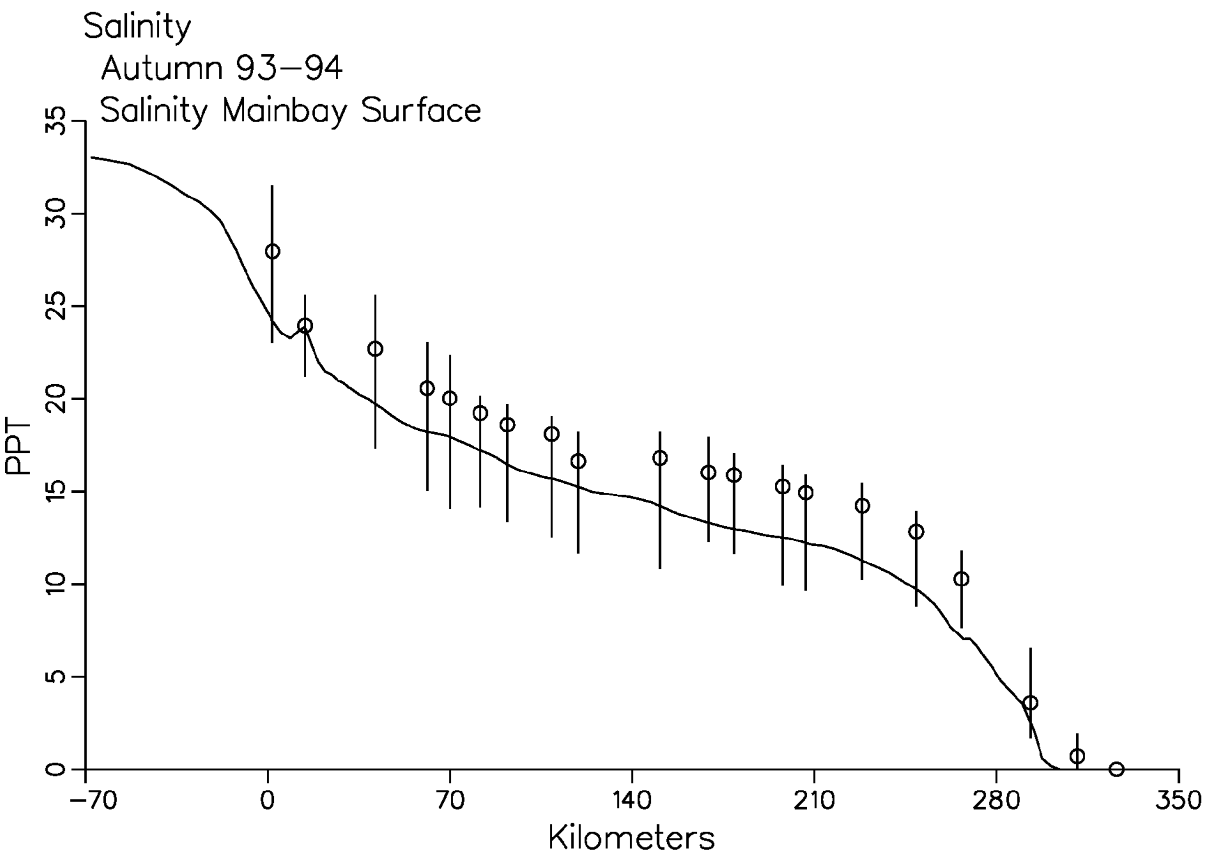
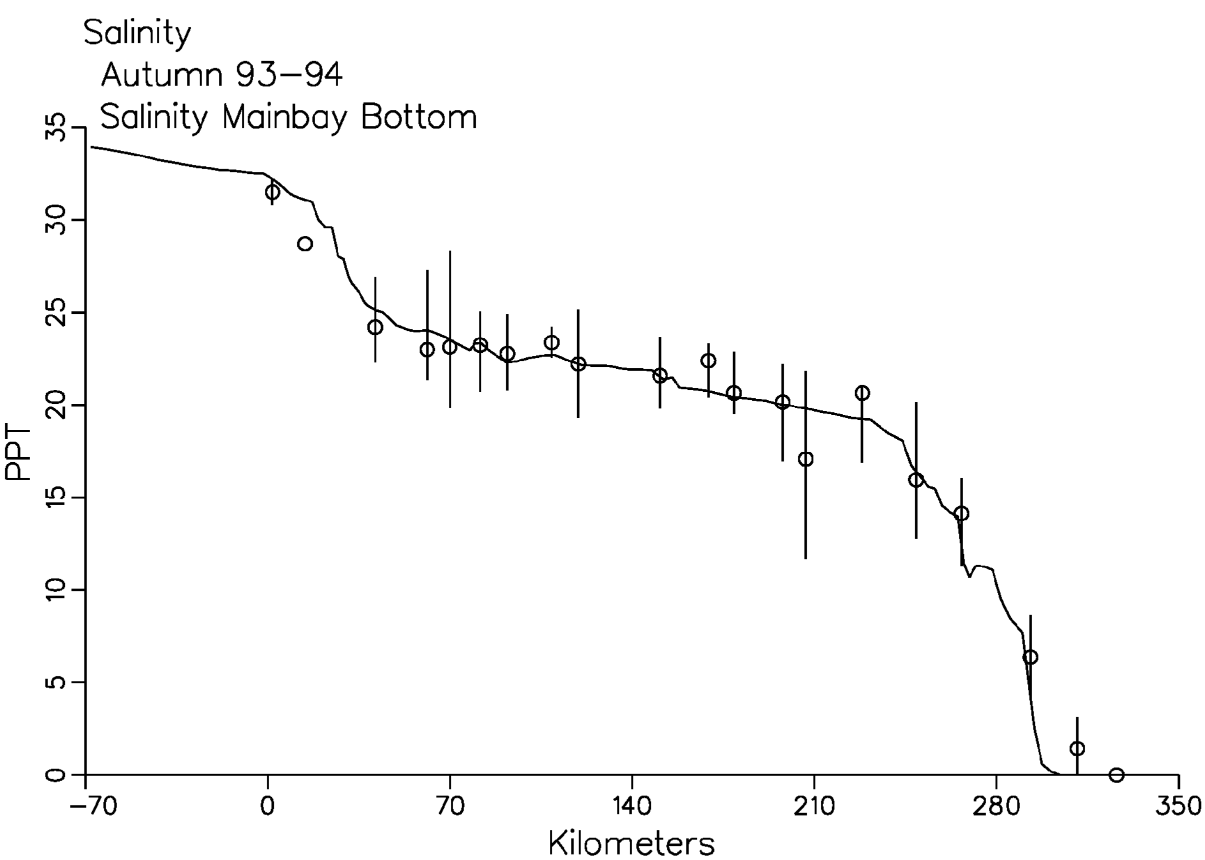
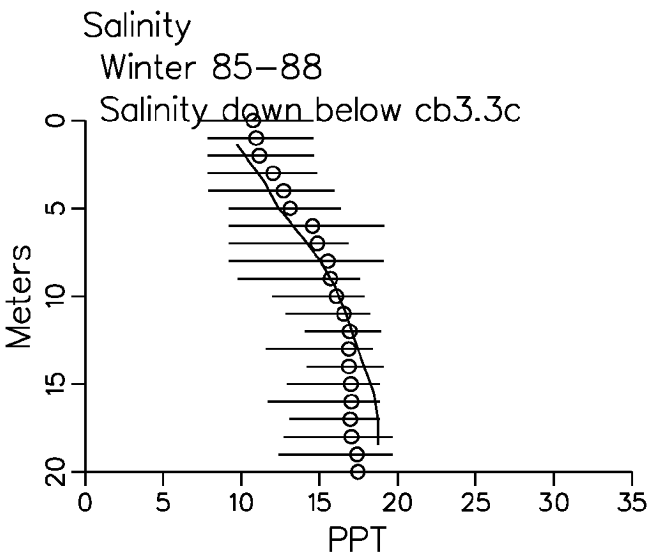
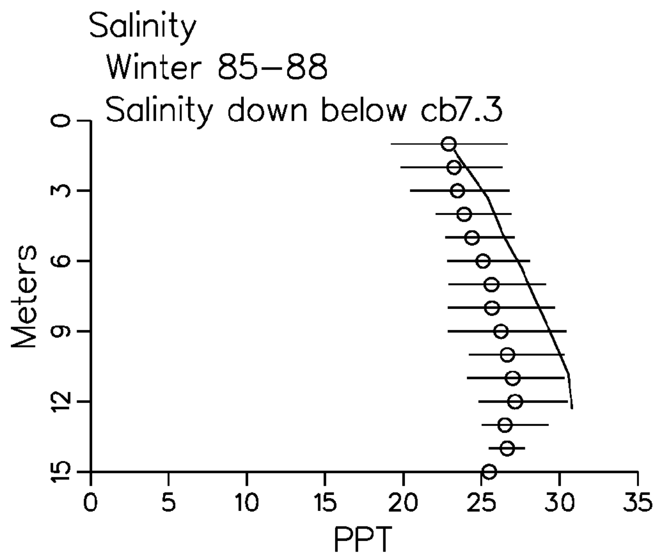
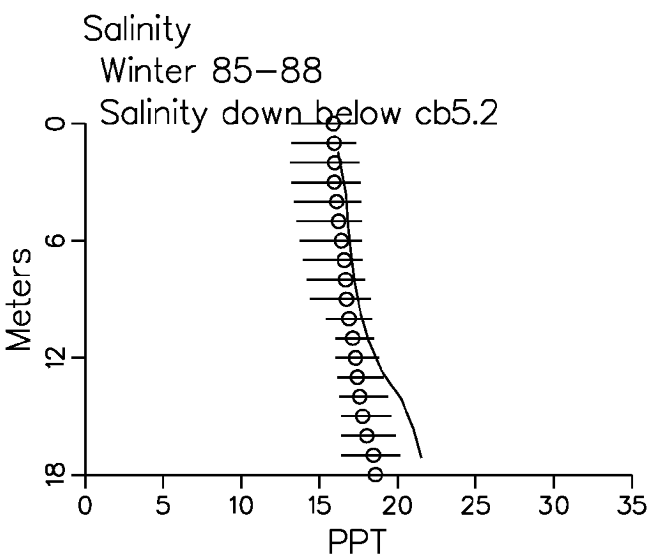


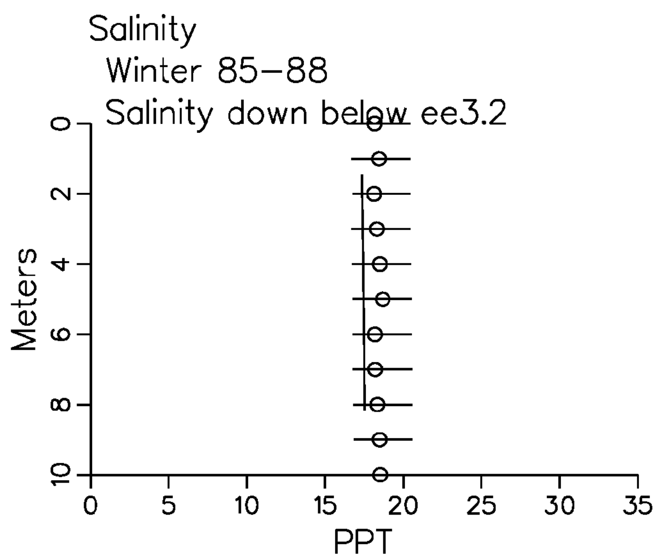


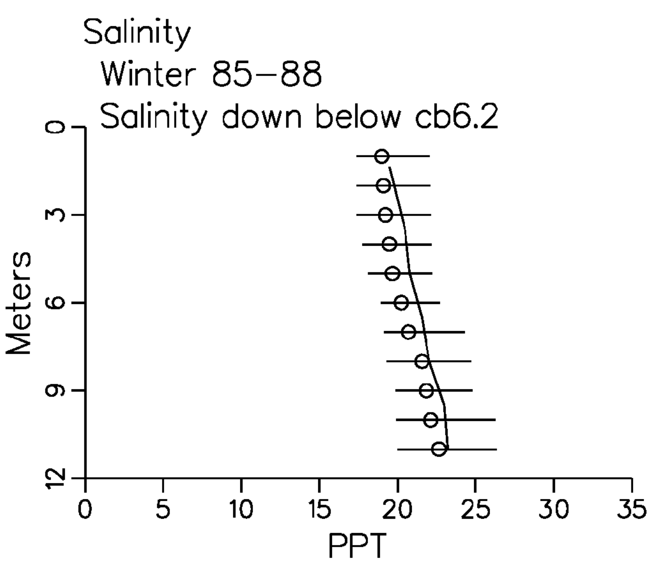
VERTICAL PROFILES, MAINSTEM BAY SALINITY 9/7/99











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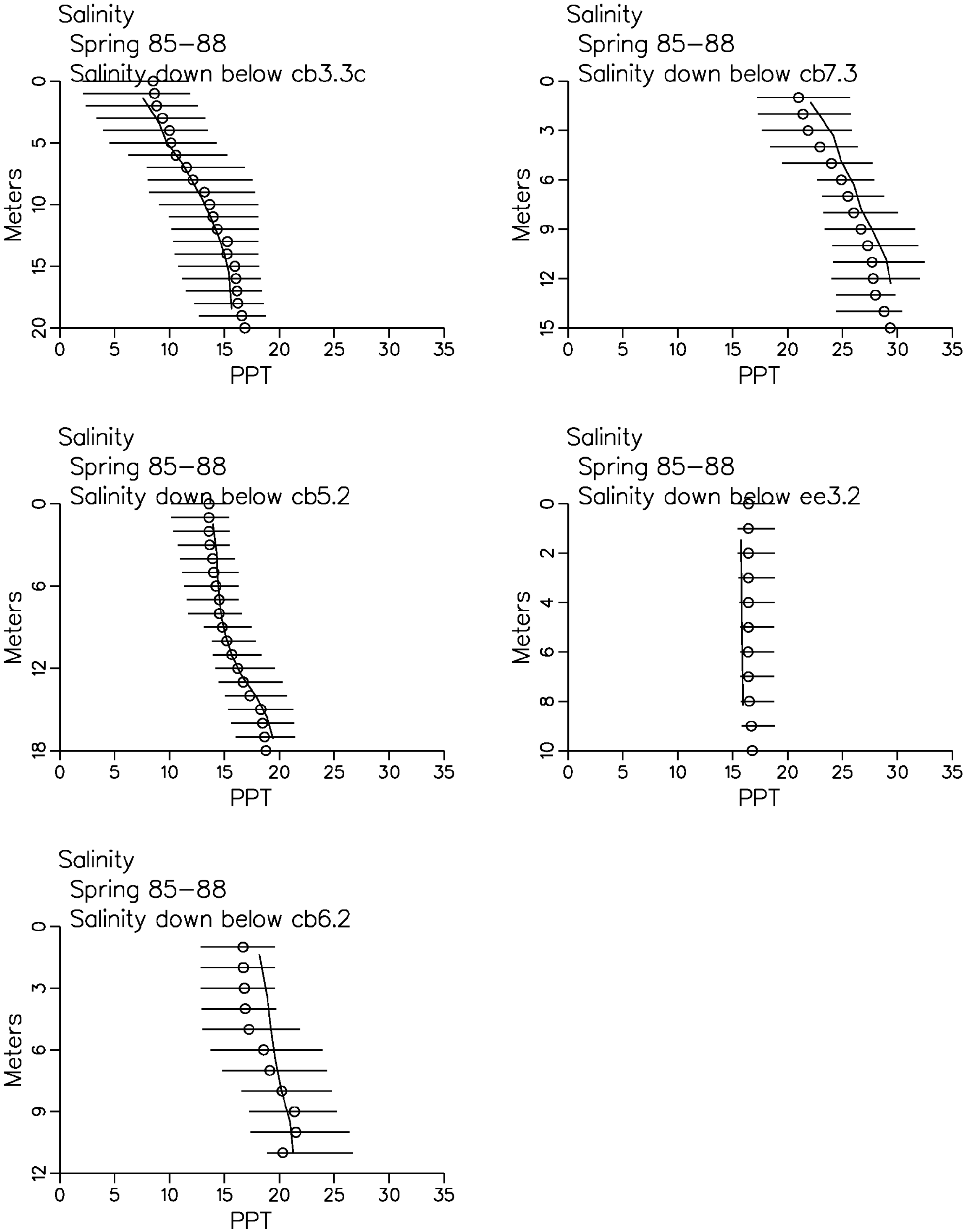

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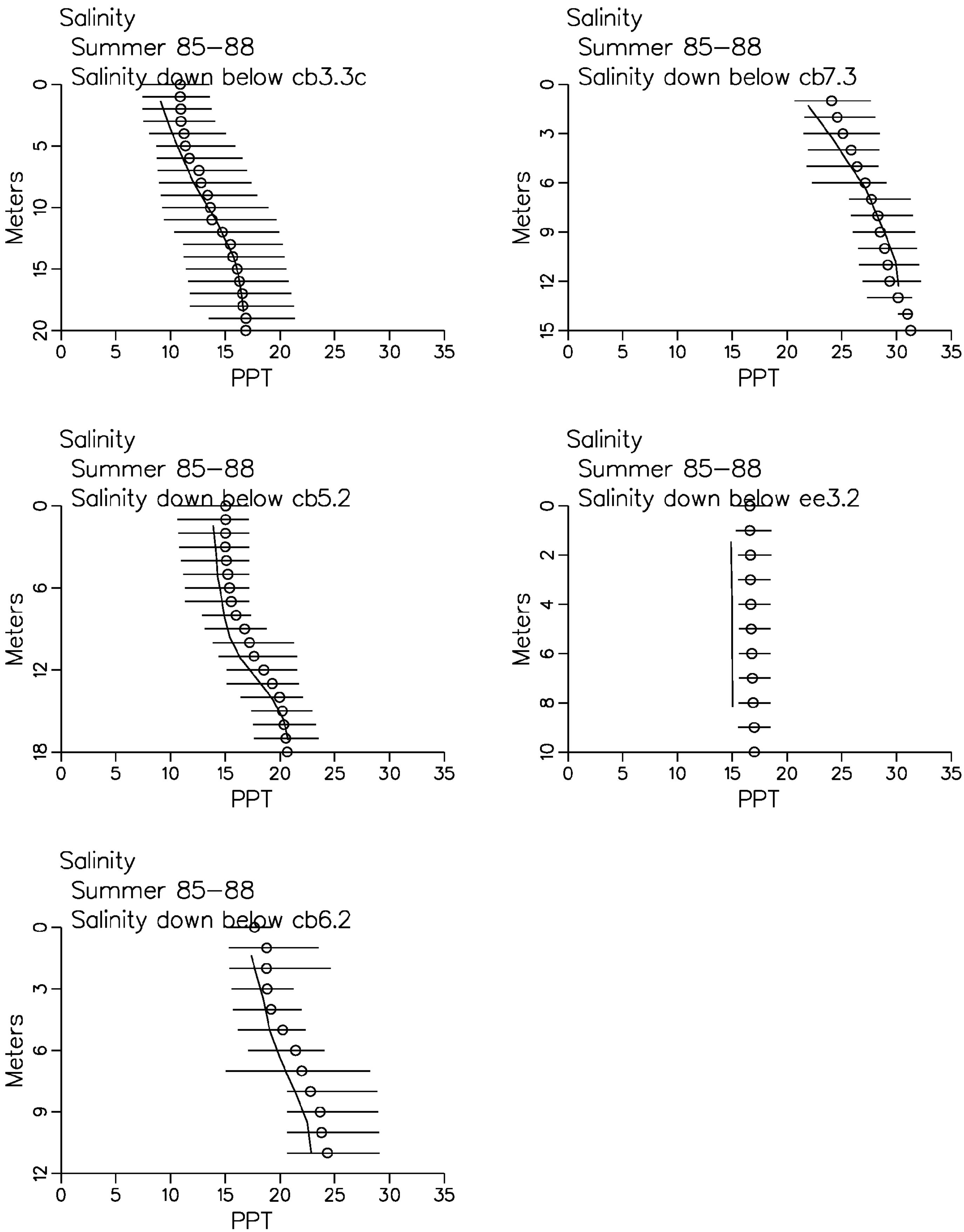

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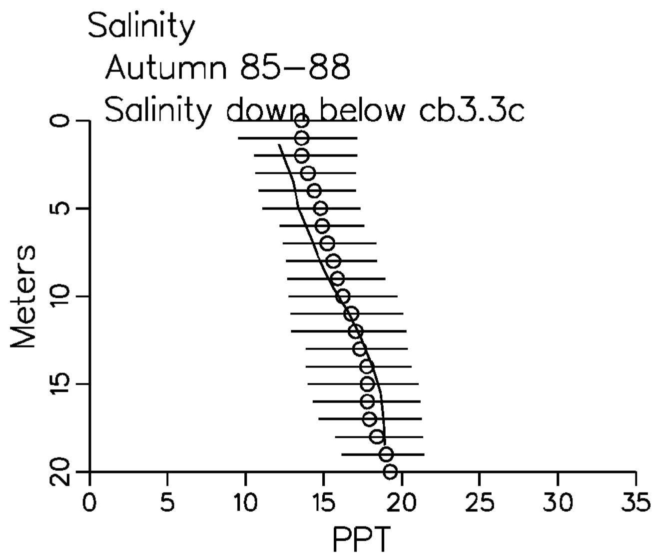

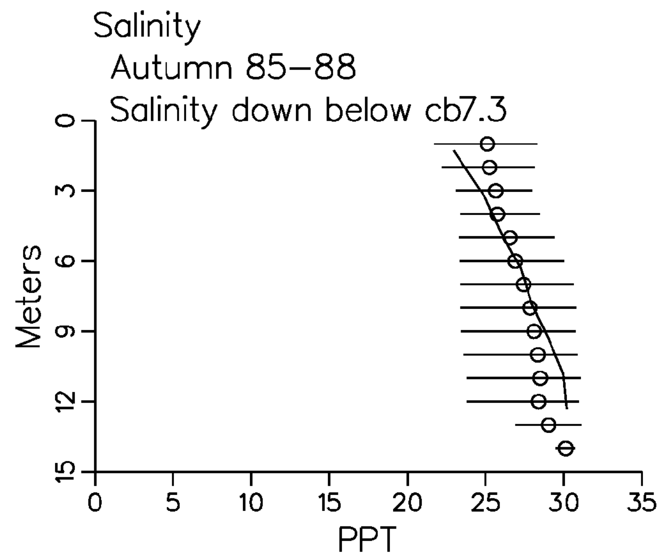

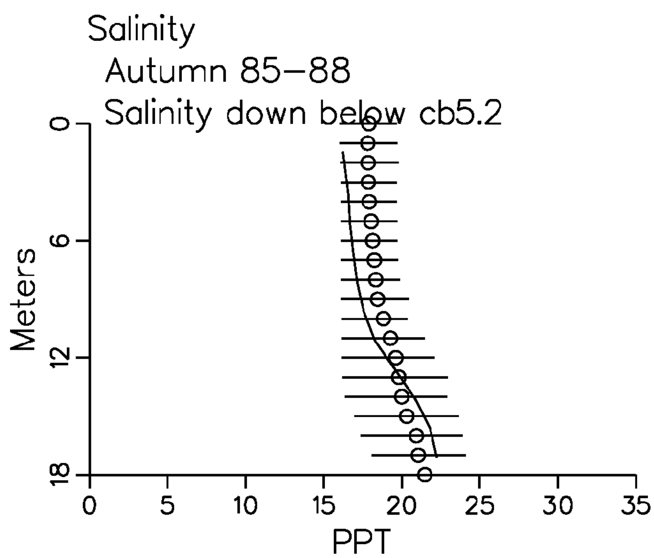

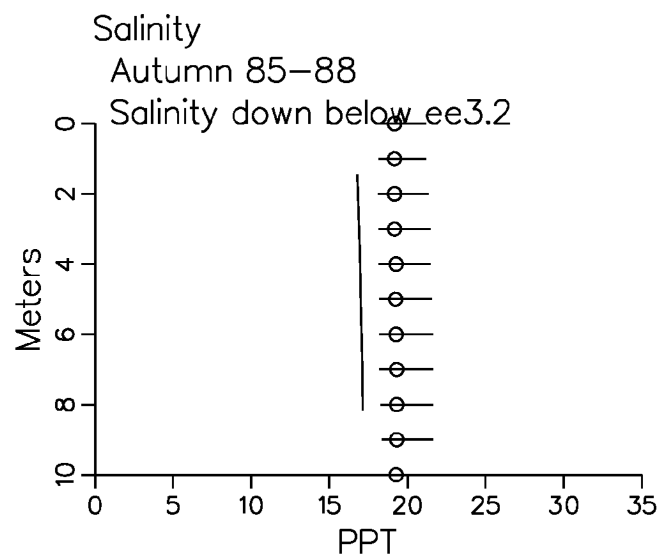

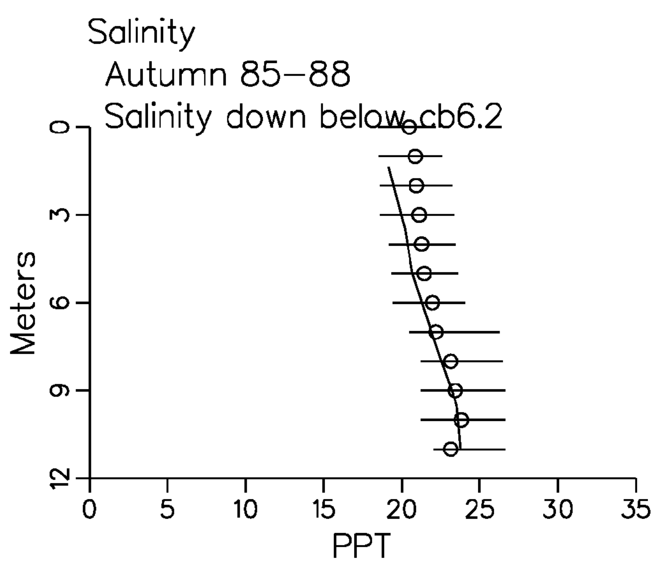

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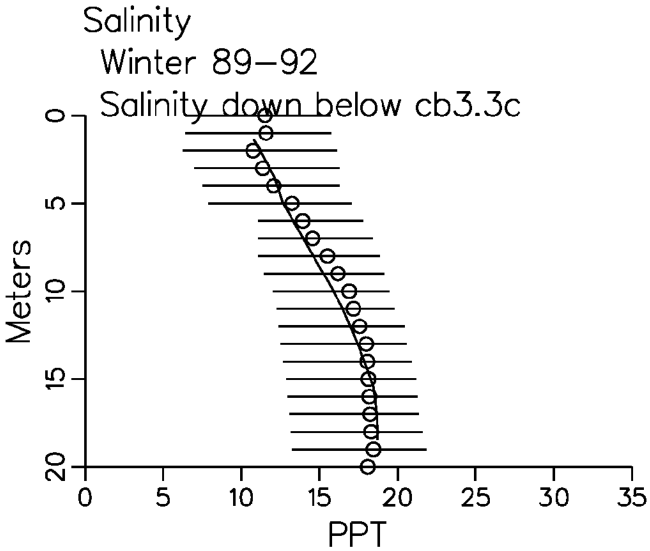

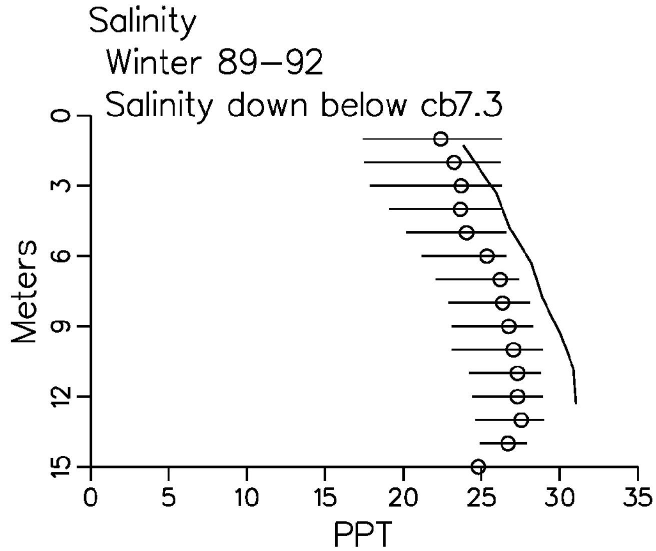

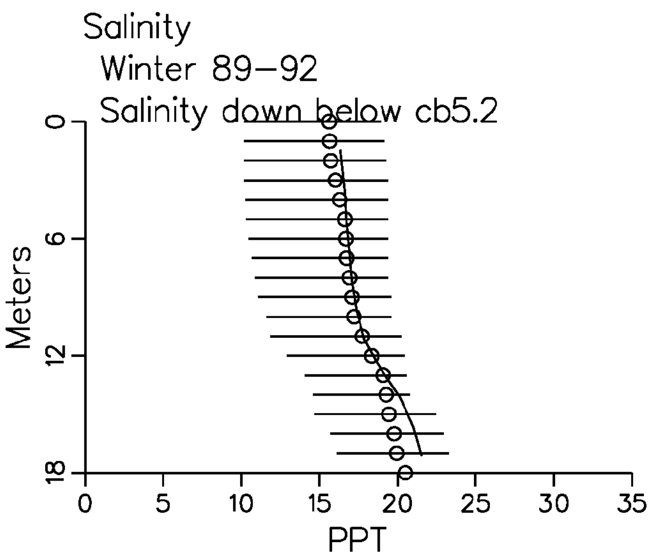

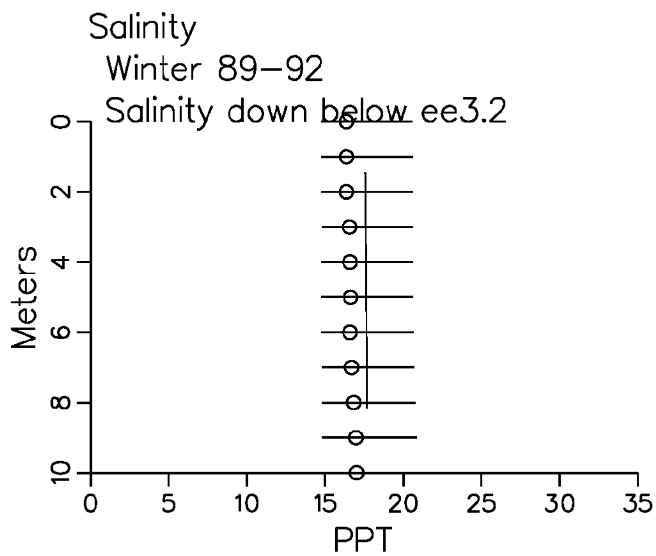

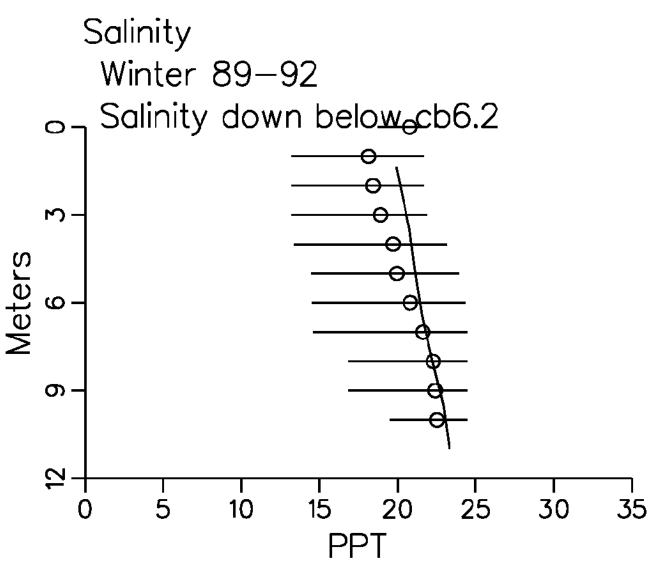

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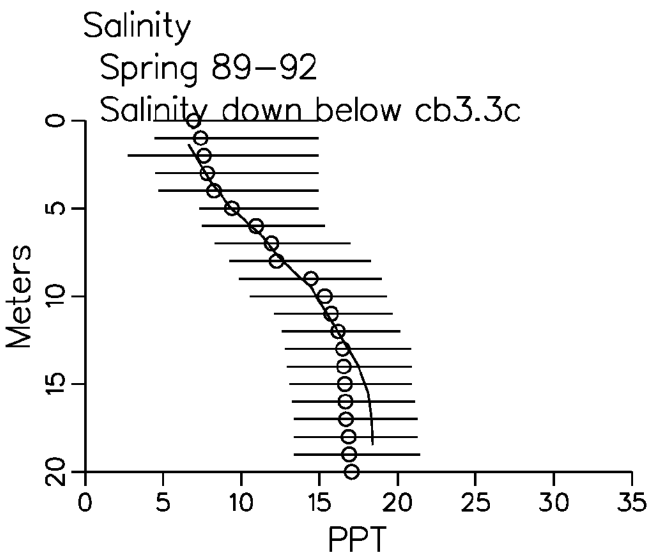

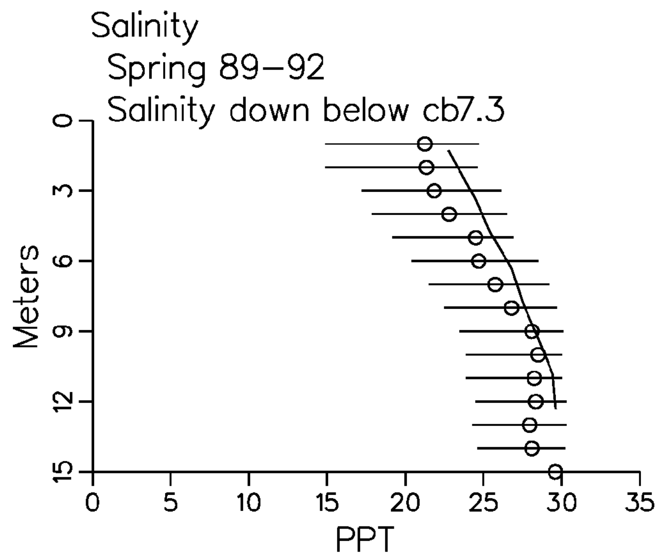

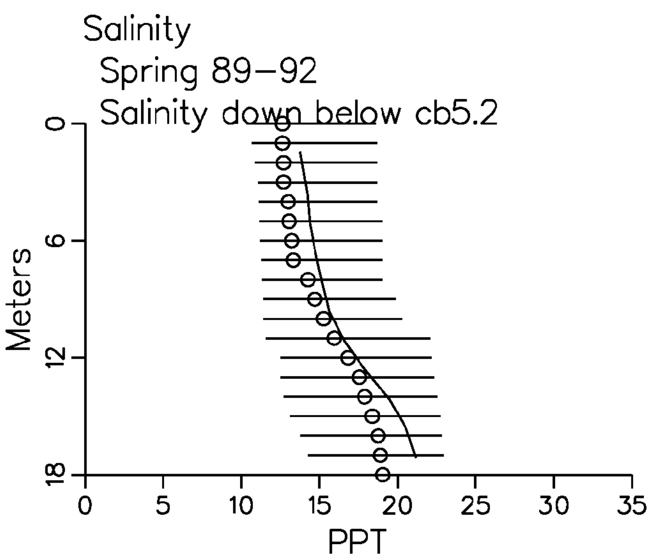

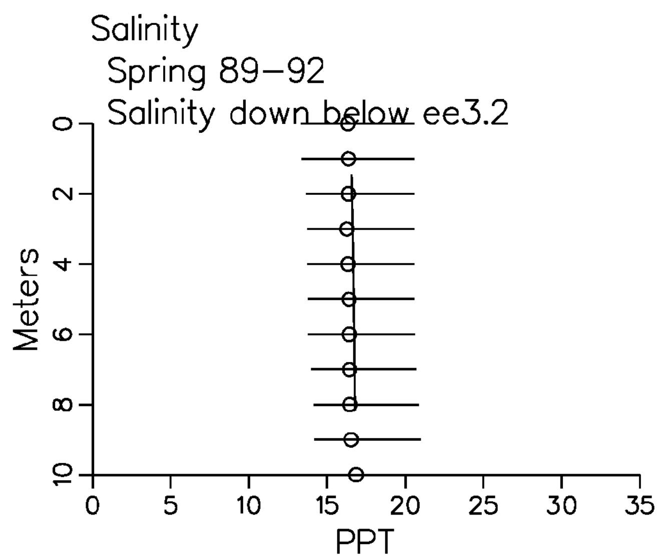

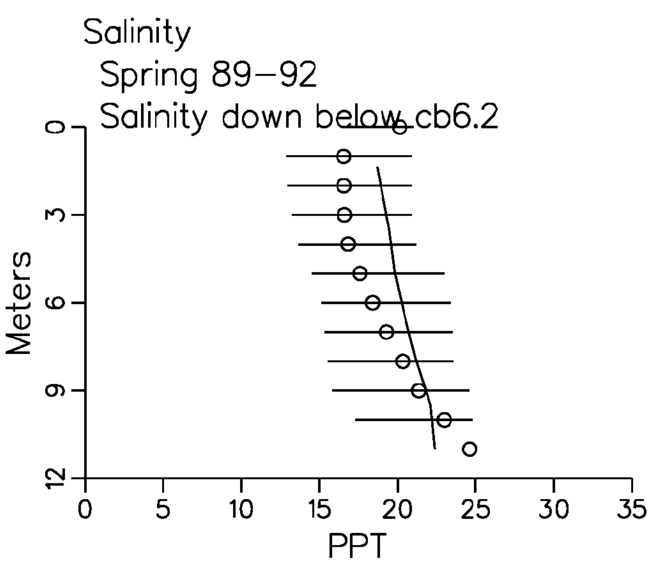

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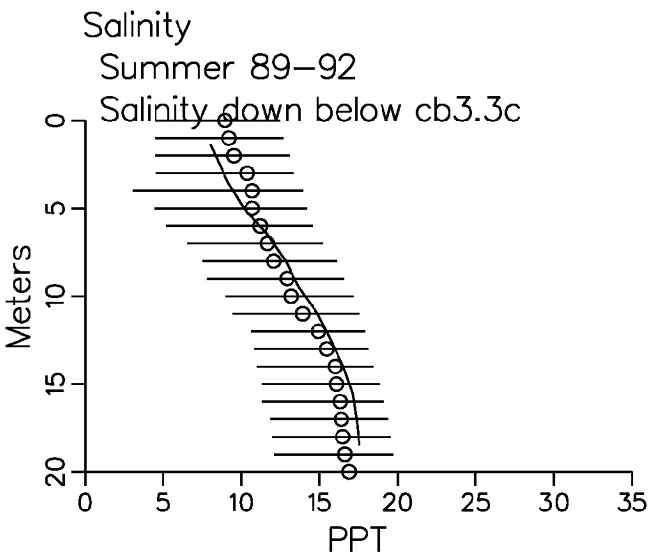

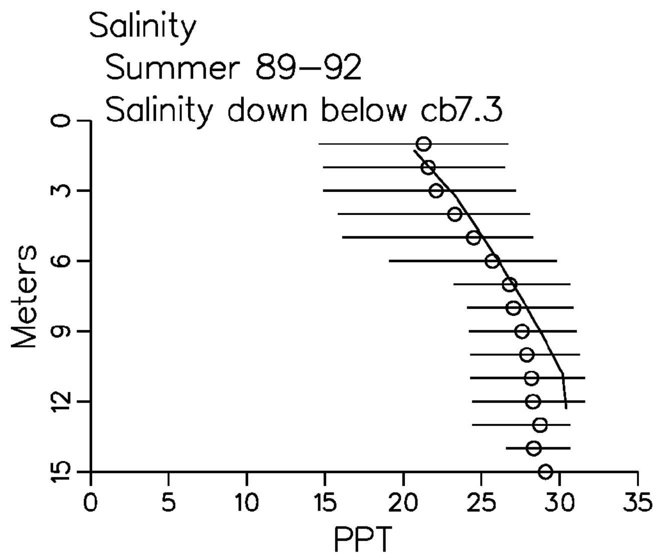

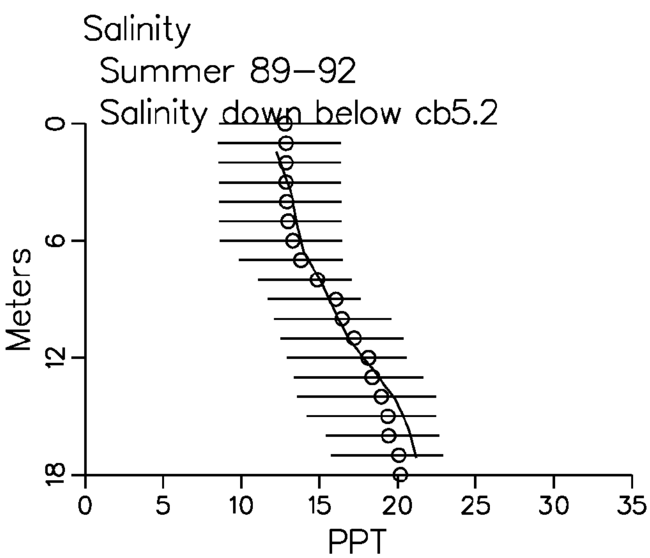

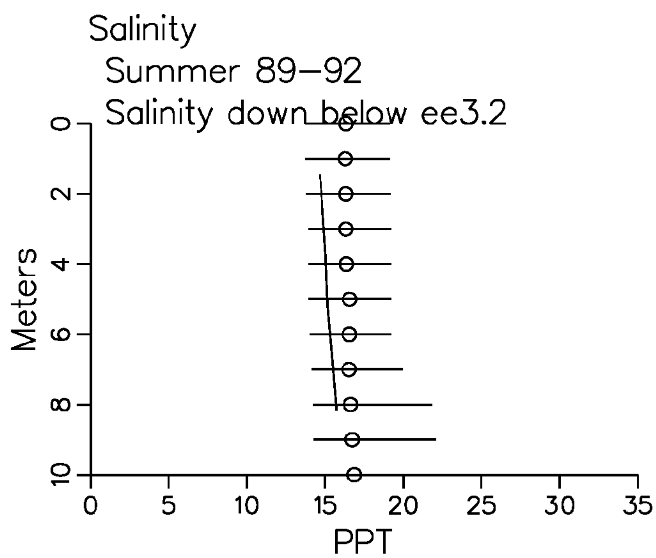

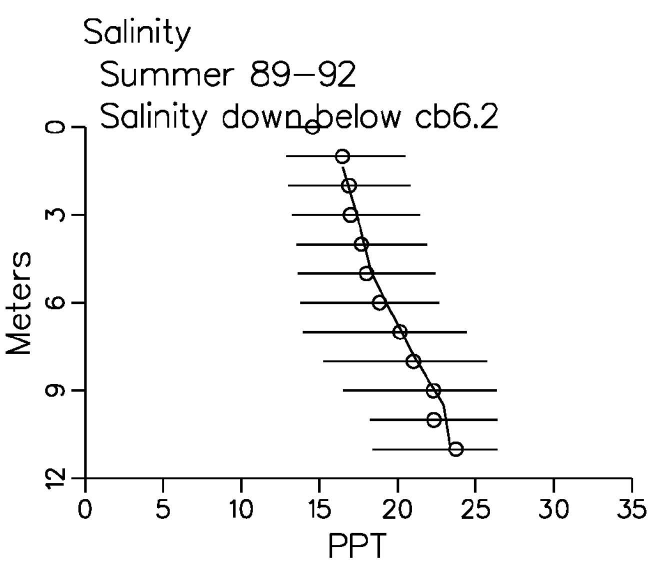

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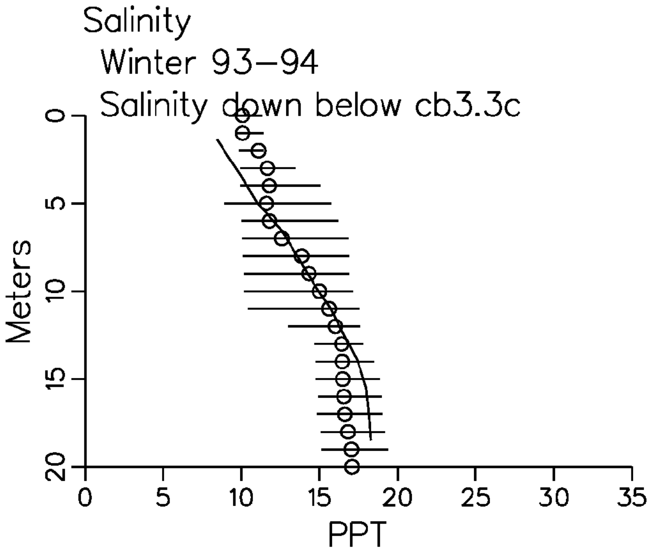

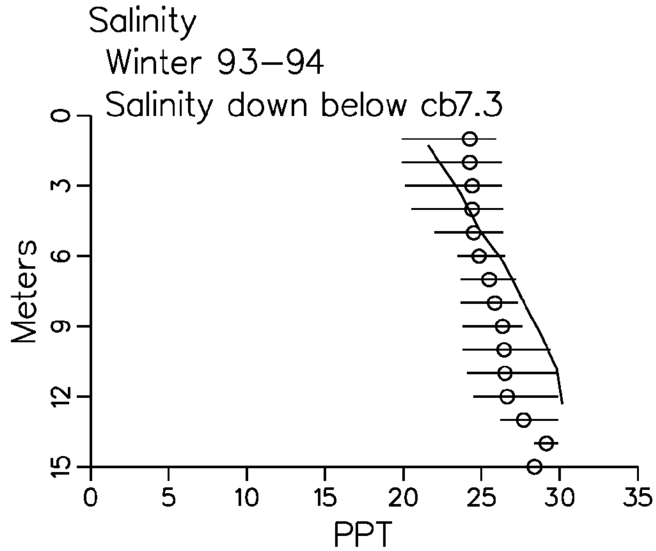

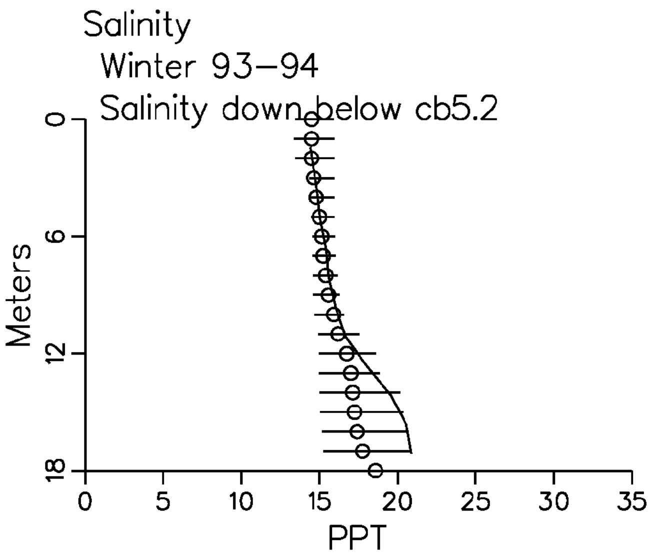

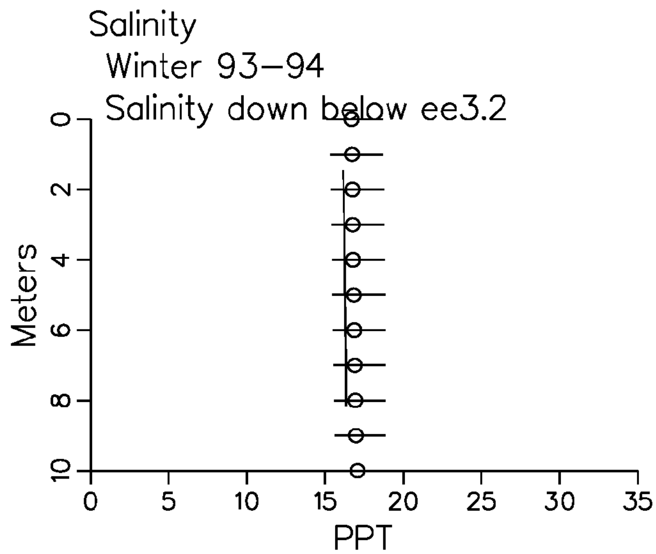

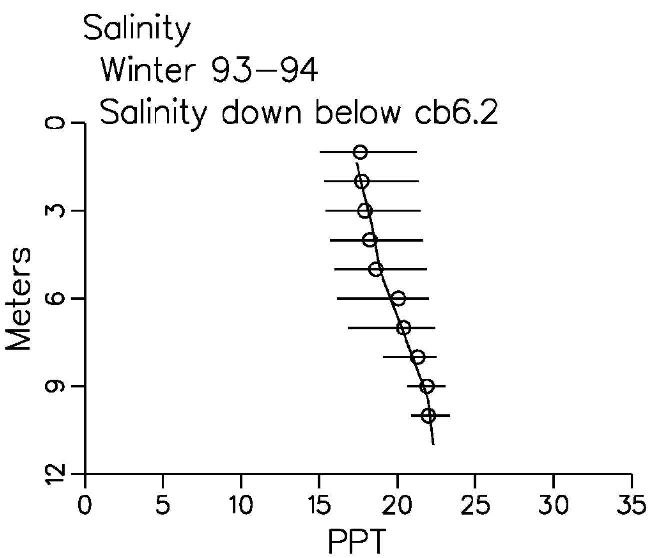

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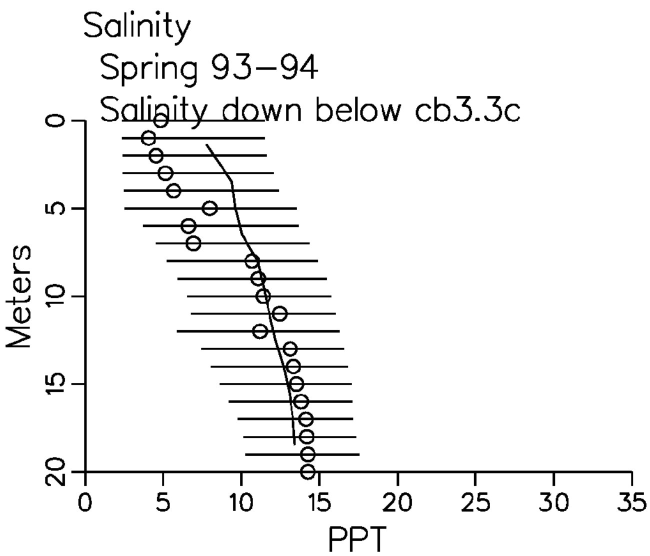

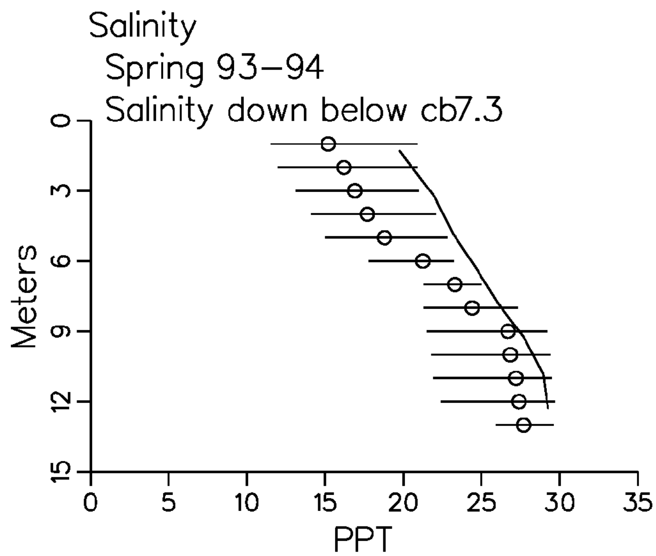

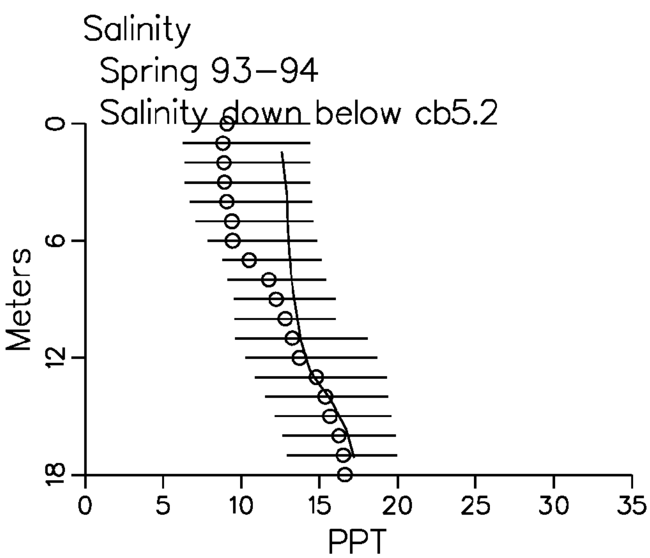

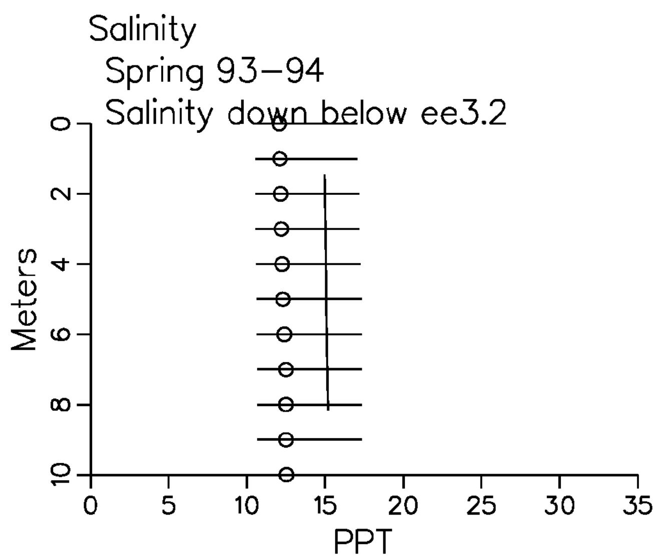

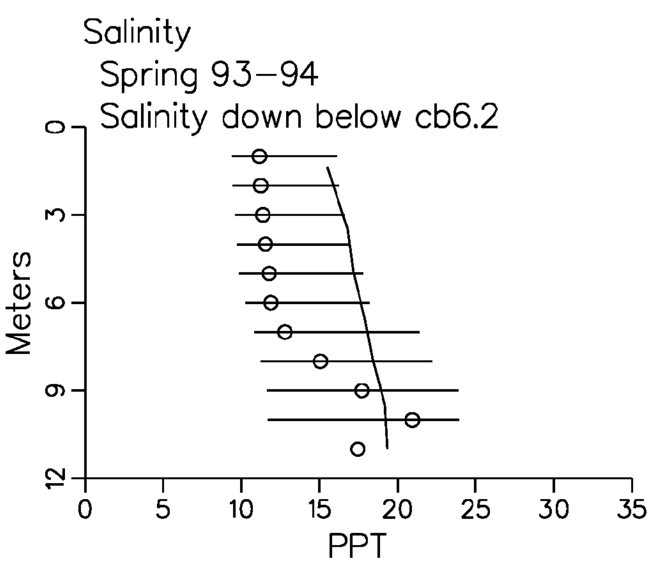

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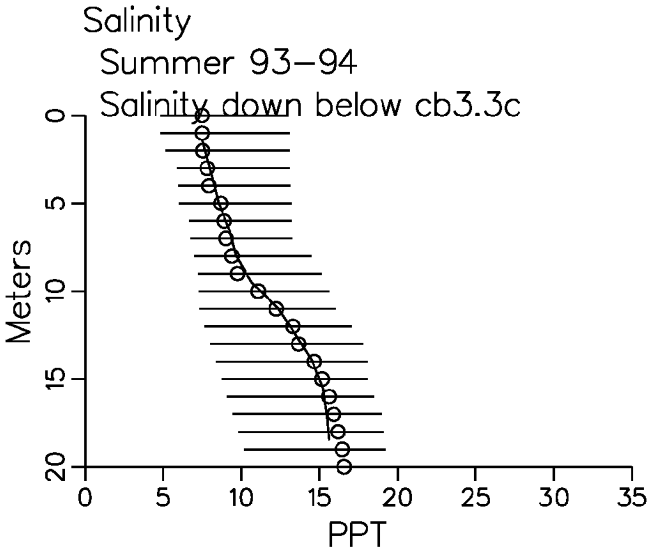

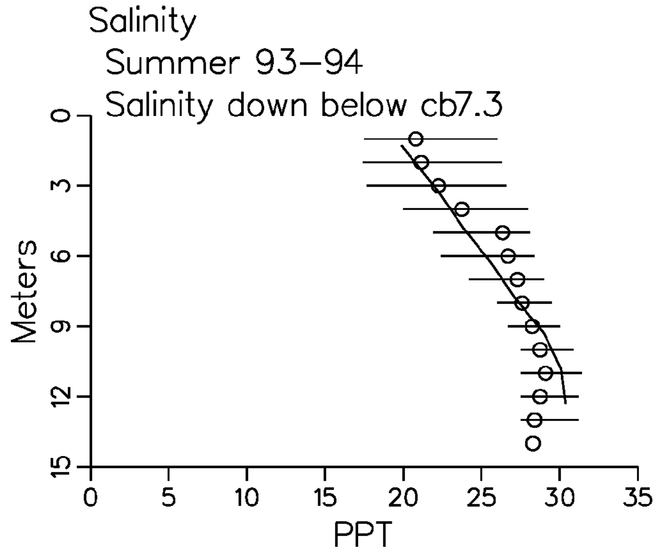

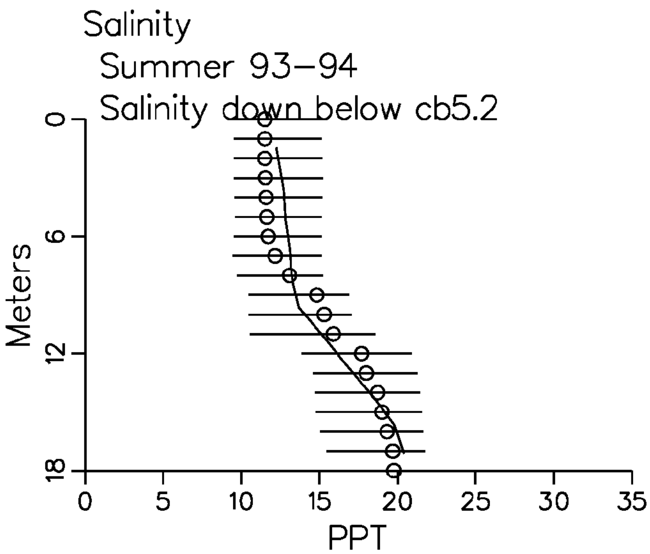

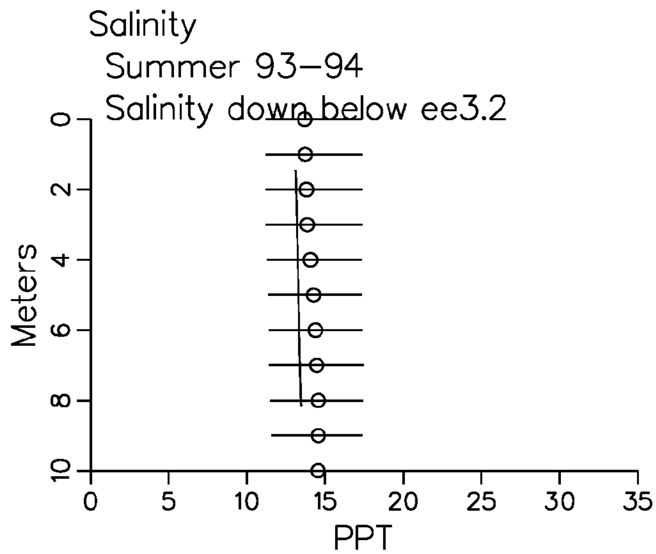

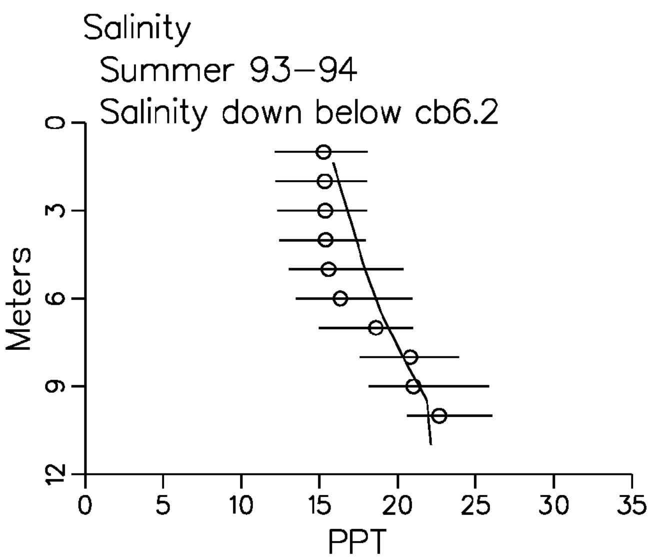

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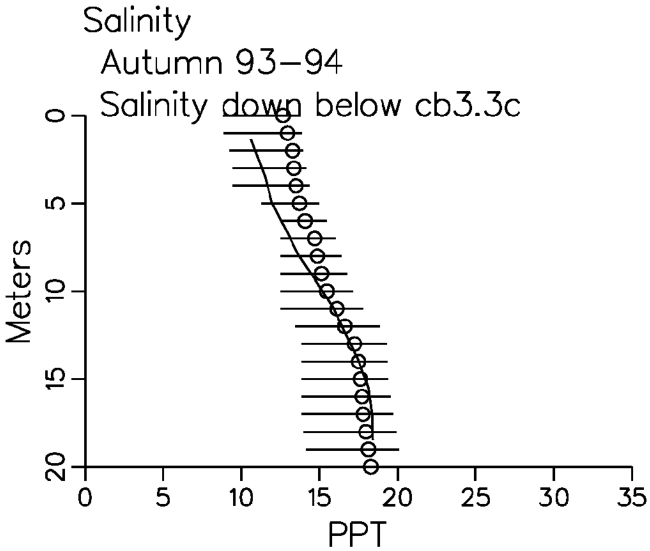
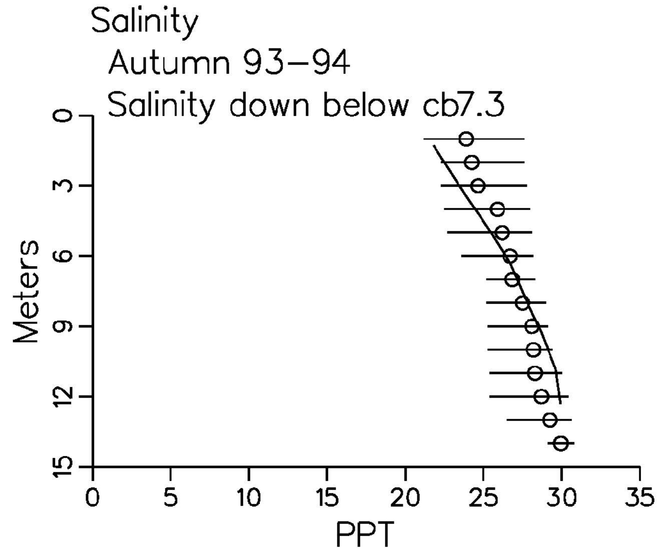
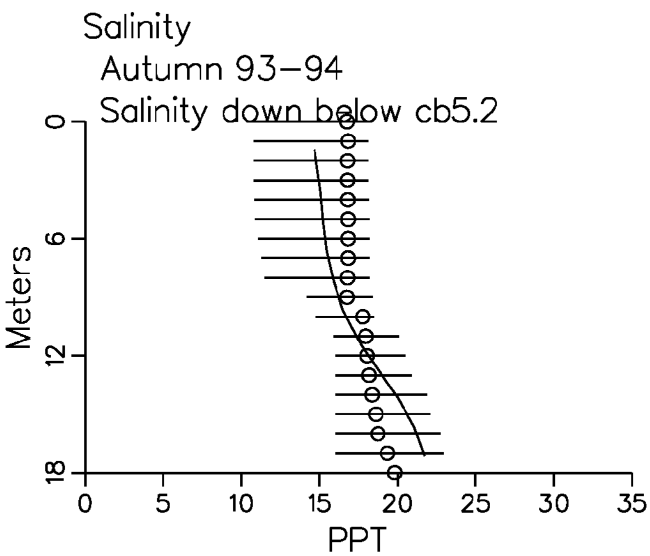
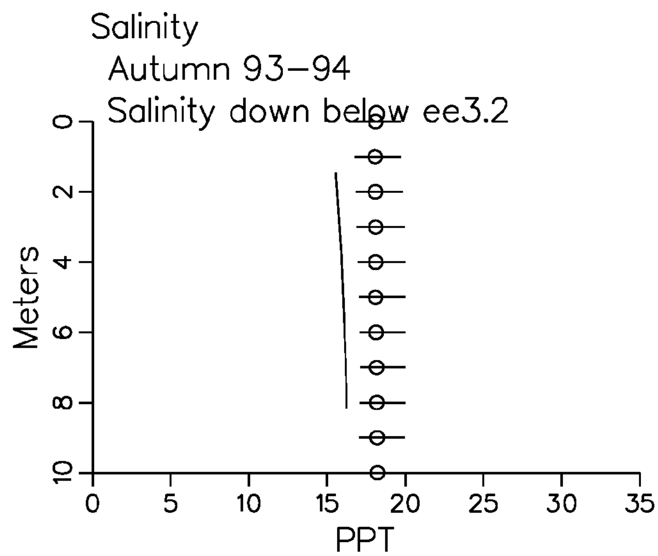
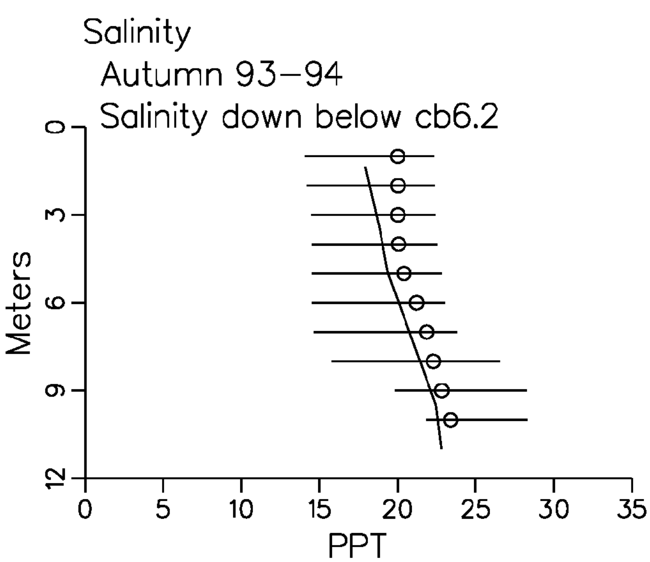


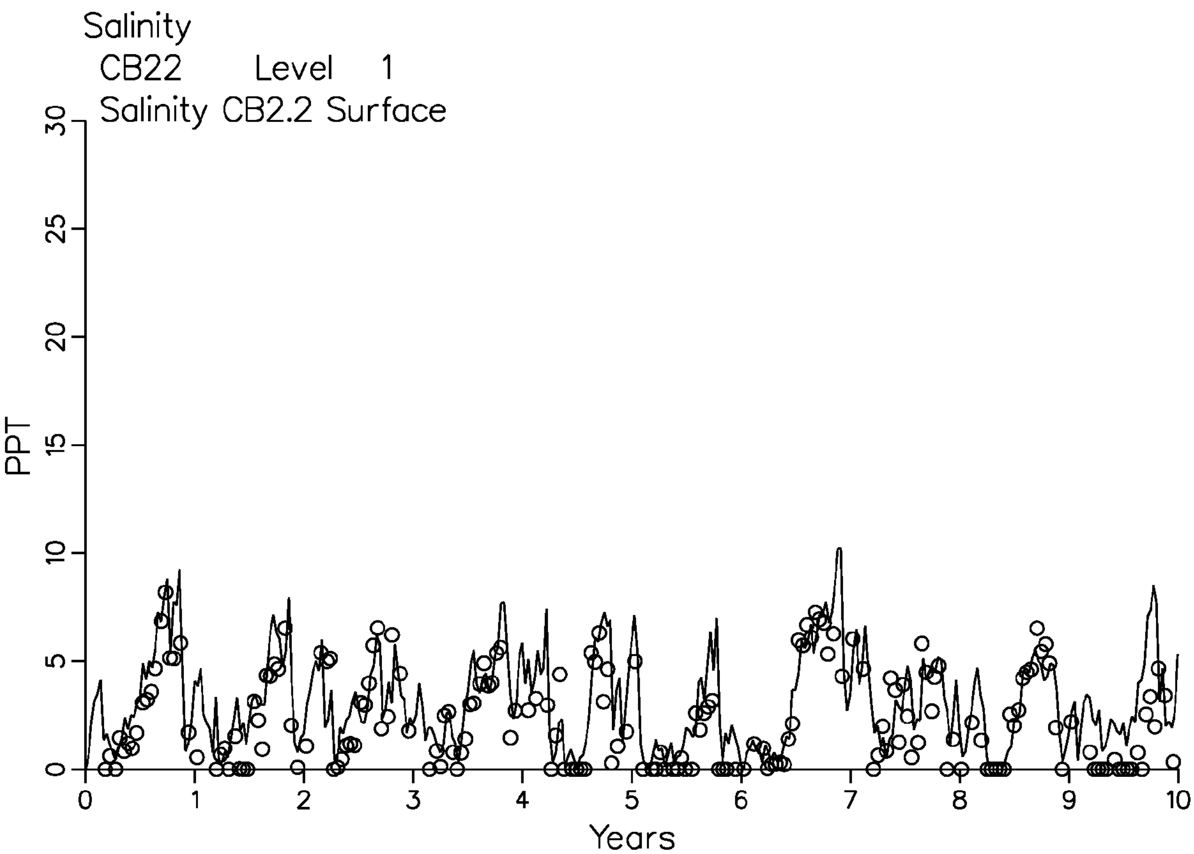


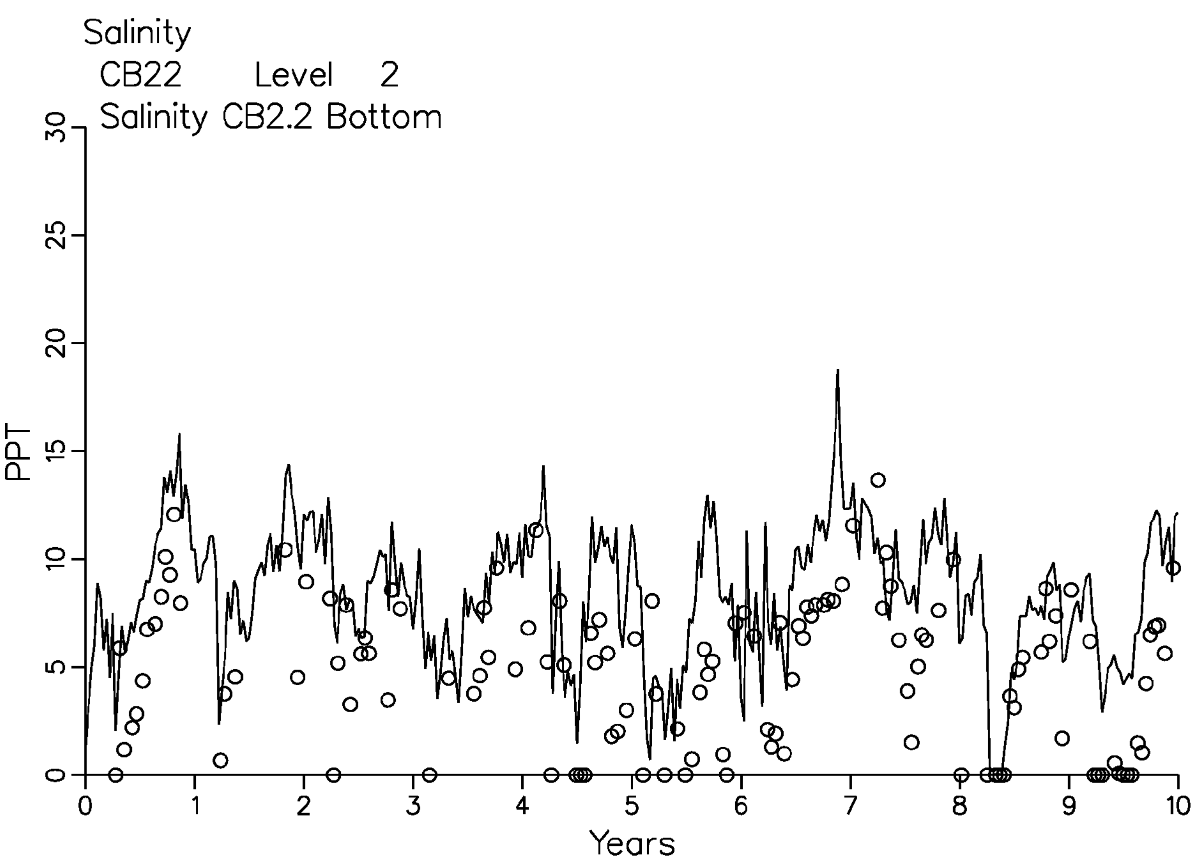






SALINITY AT SELECTED STATIONS IN MAINSTEM BAY 9/7/99





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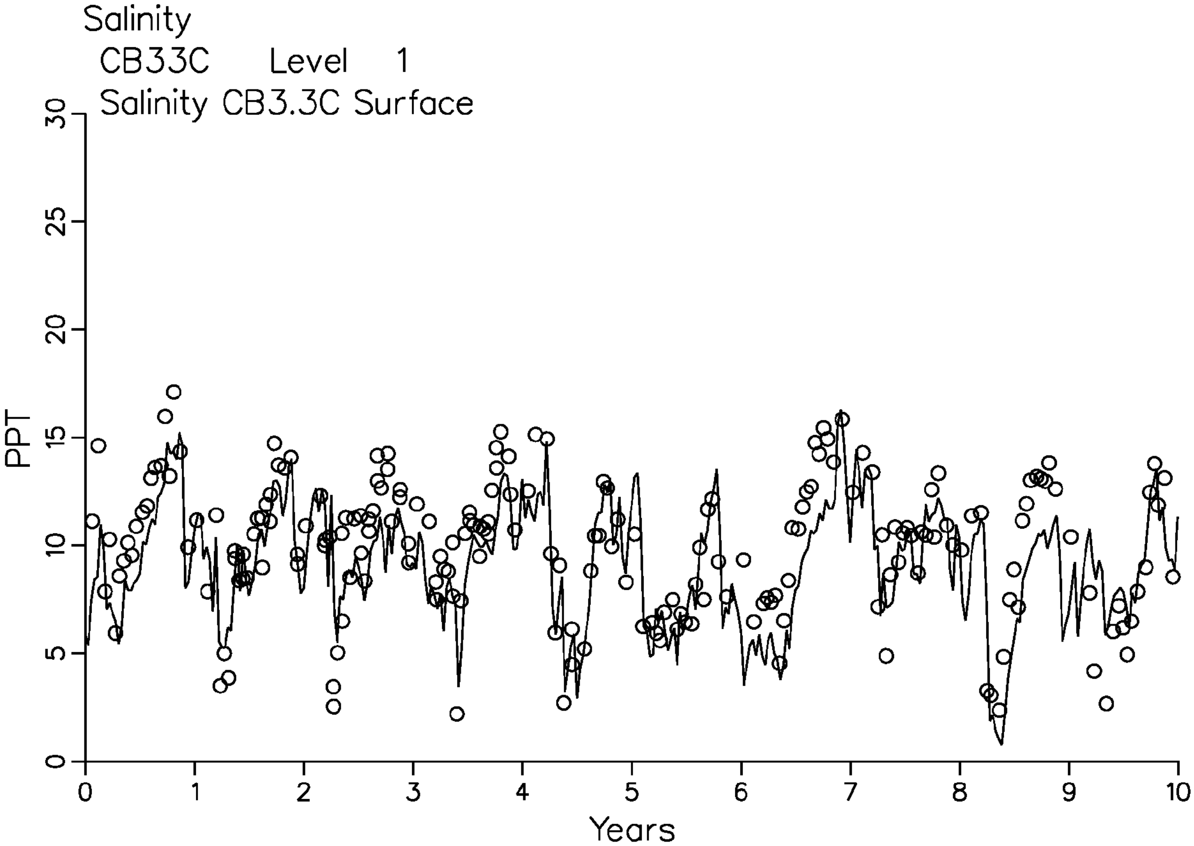

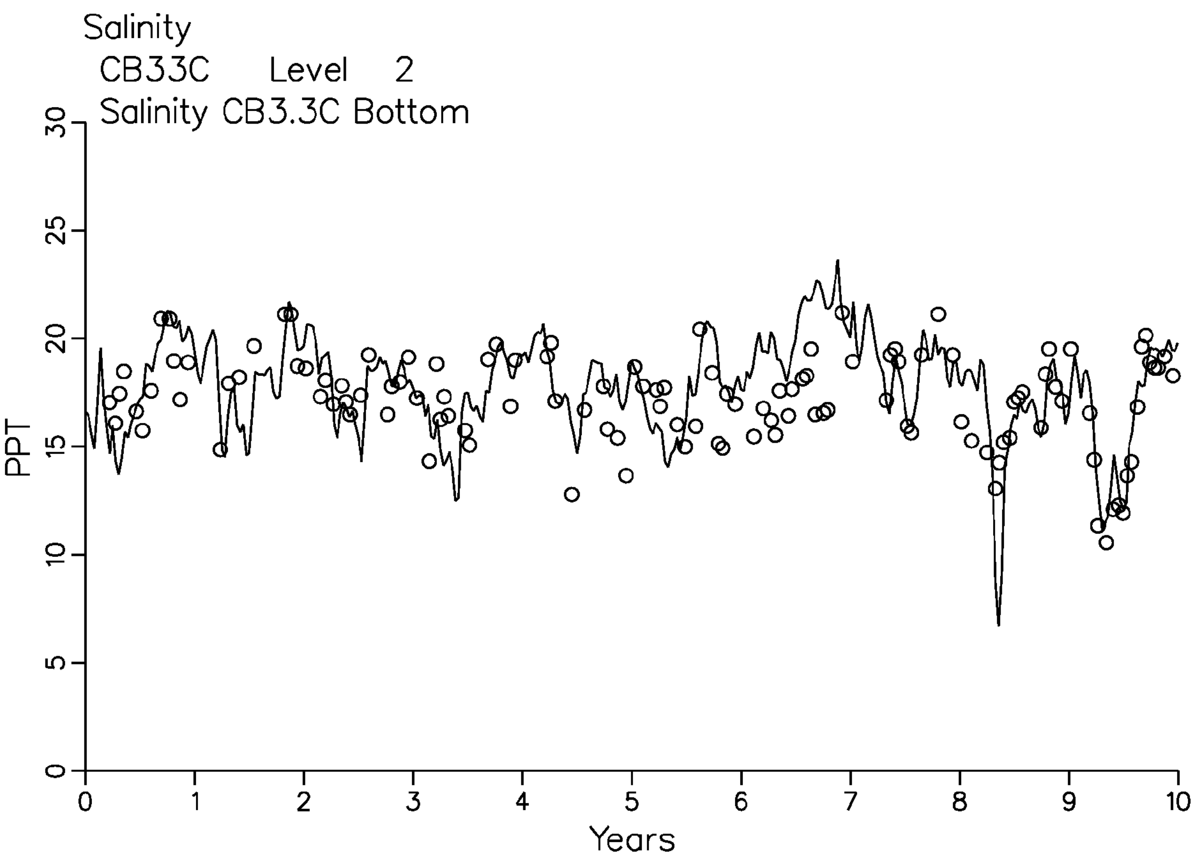

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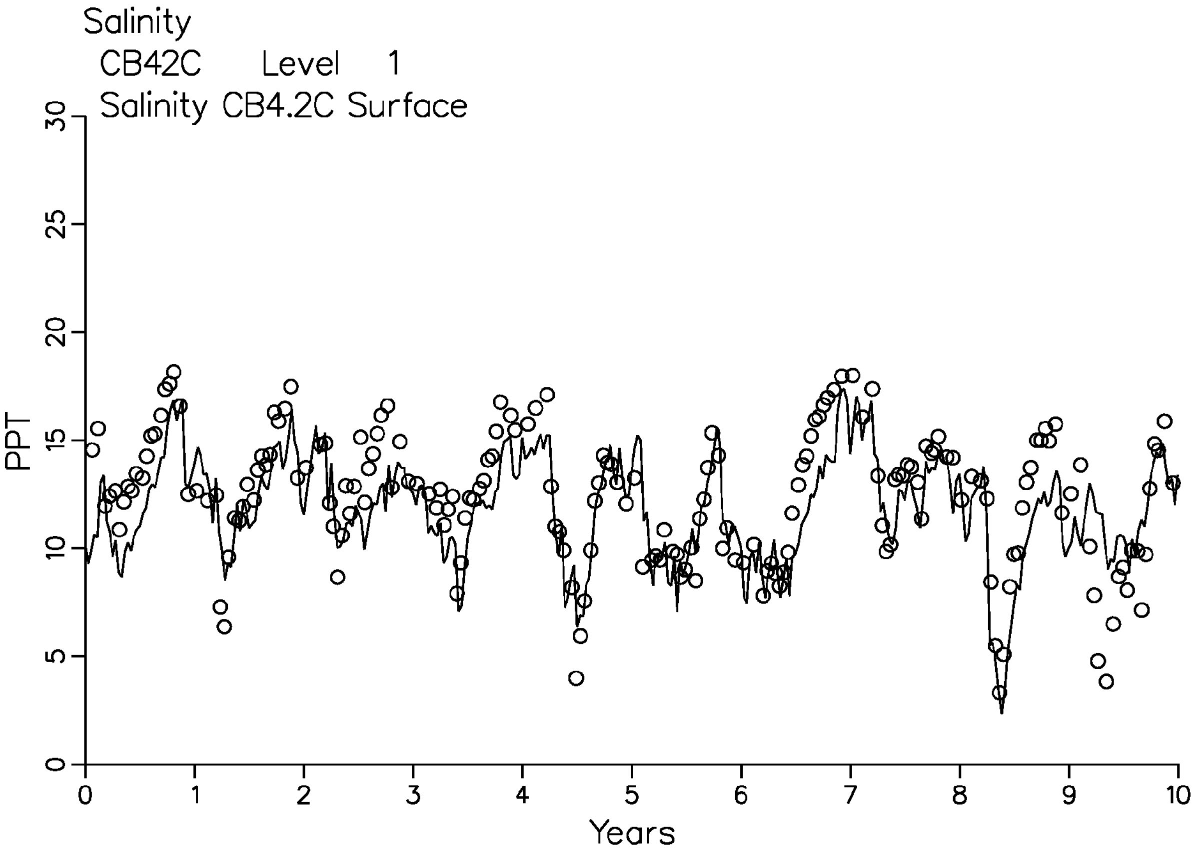

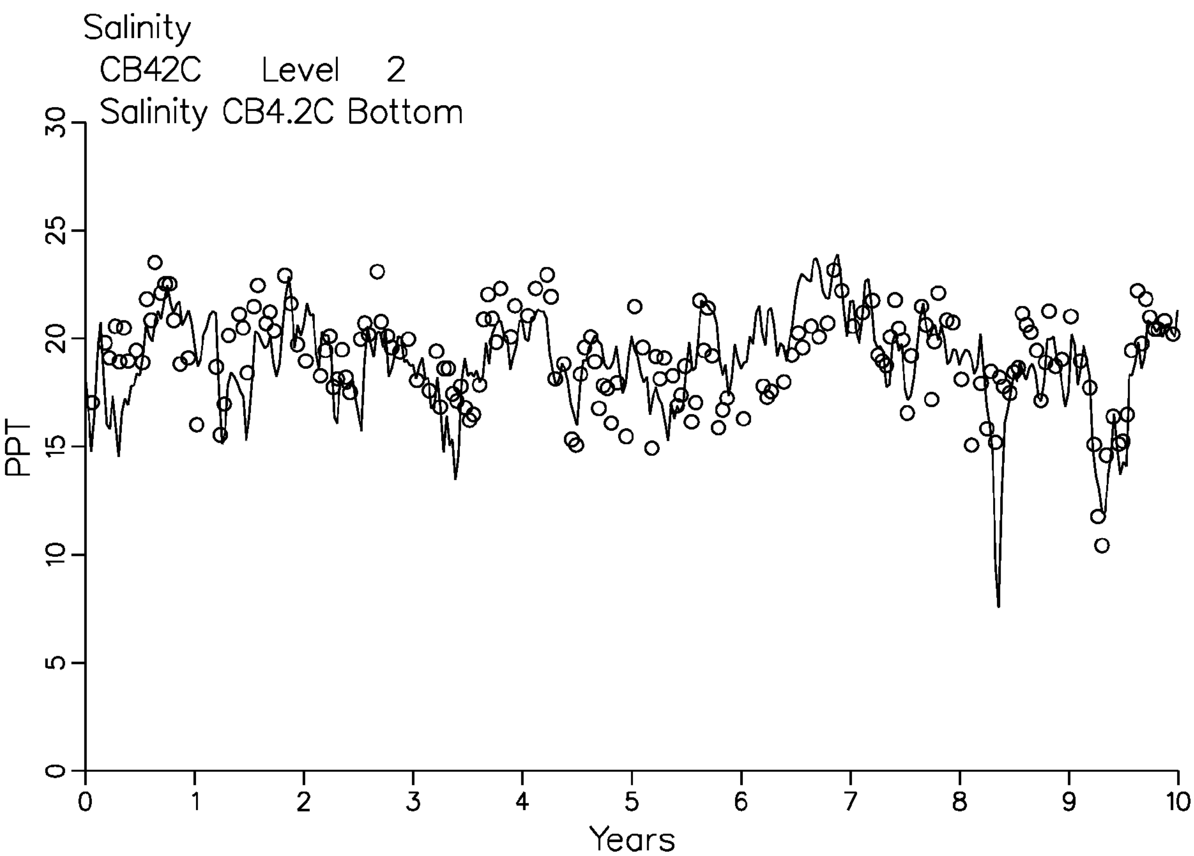

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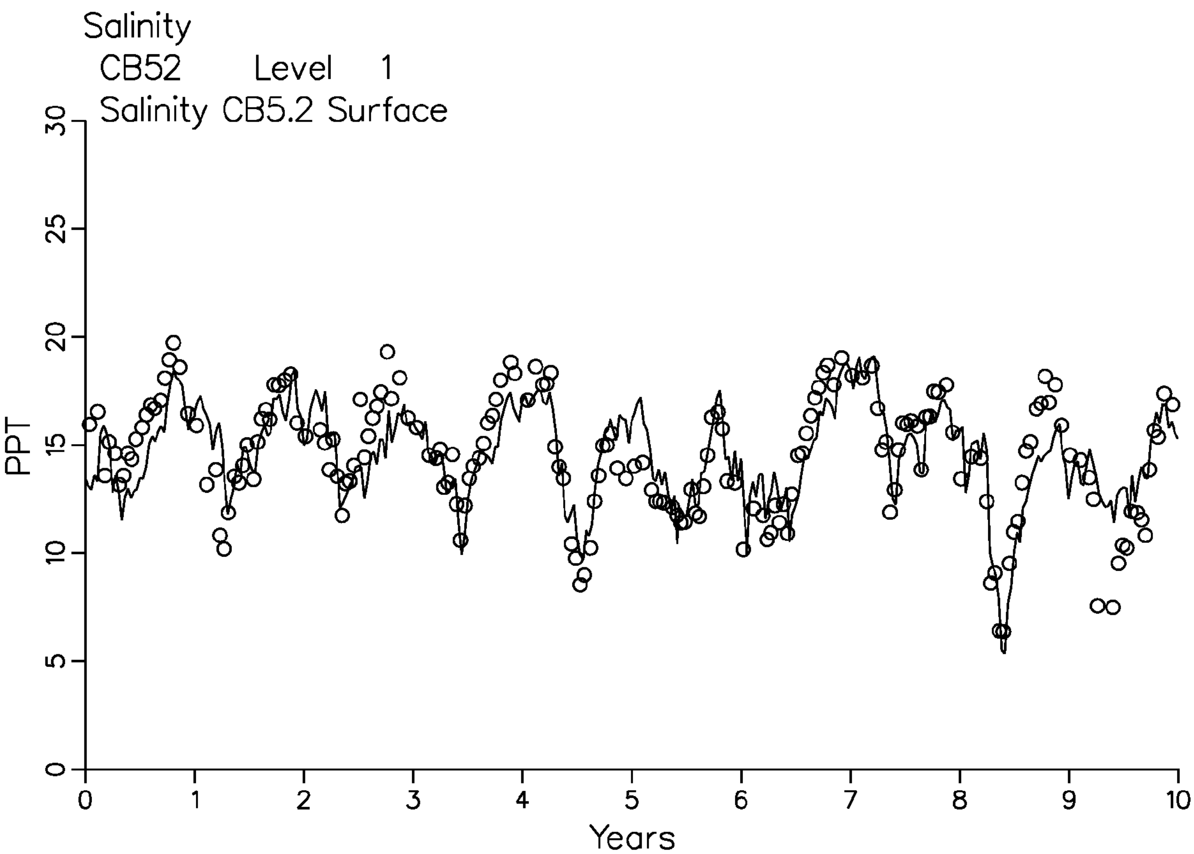

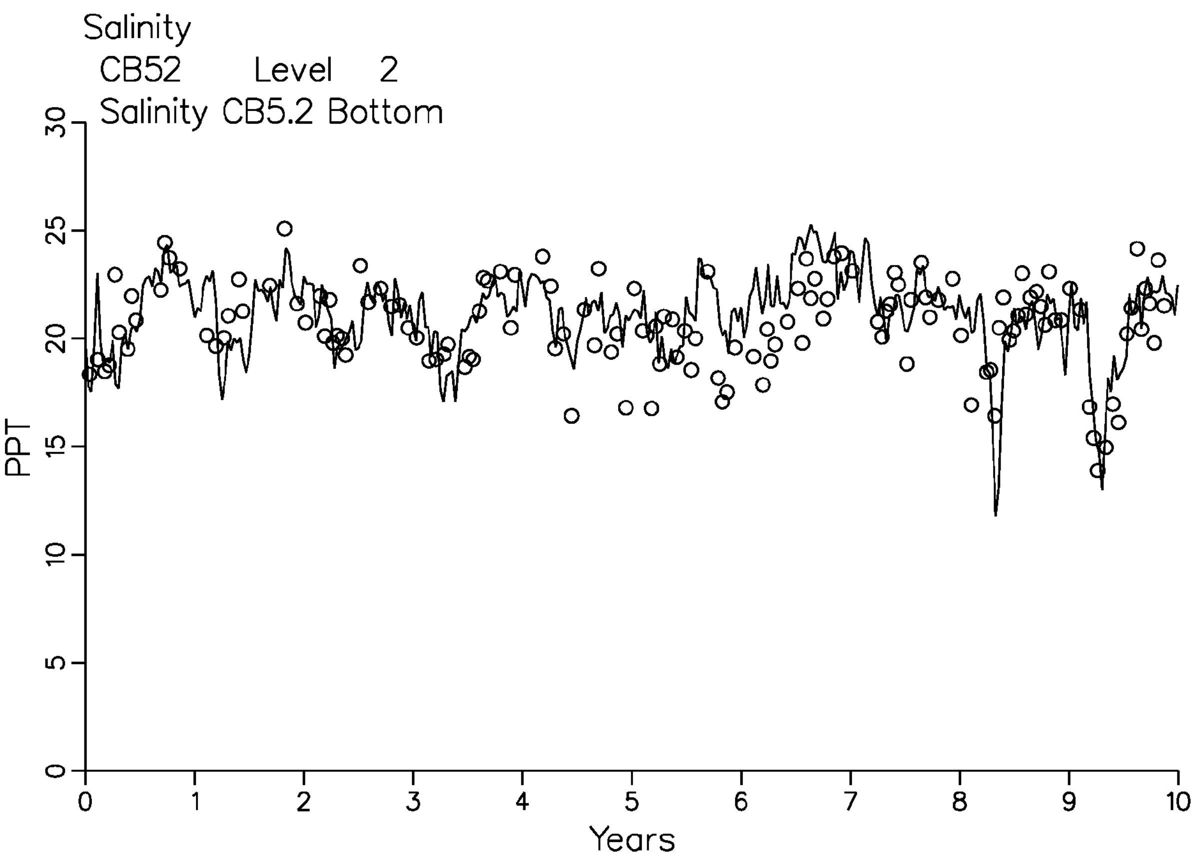

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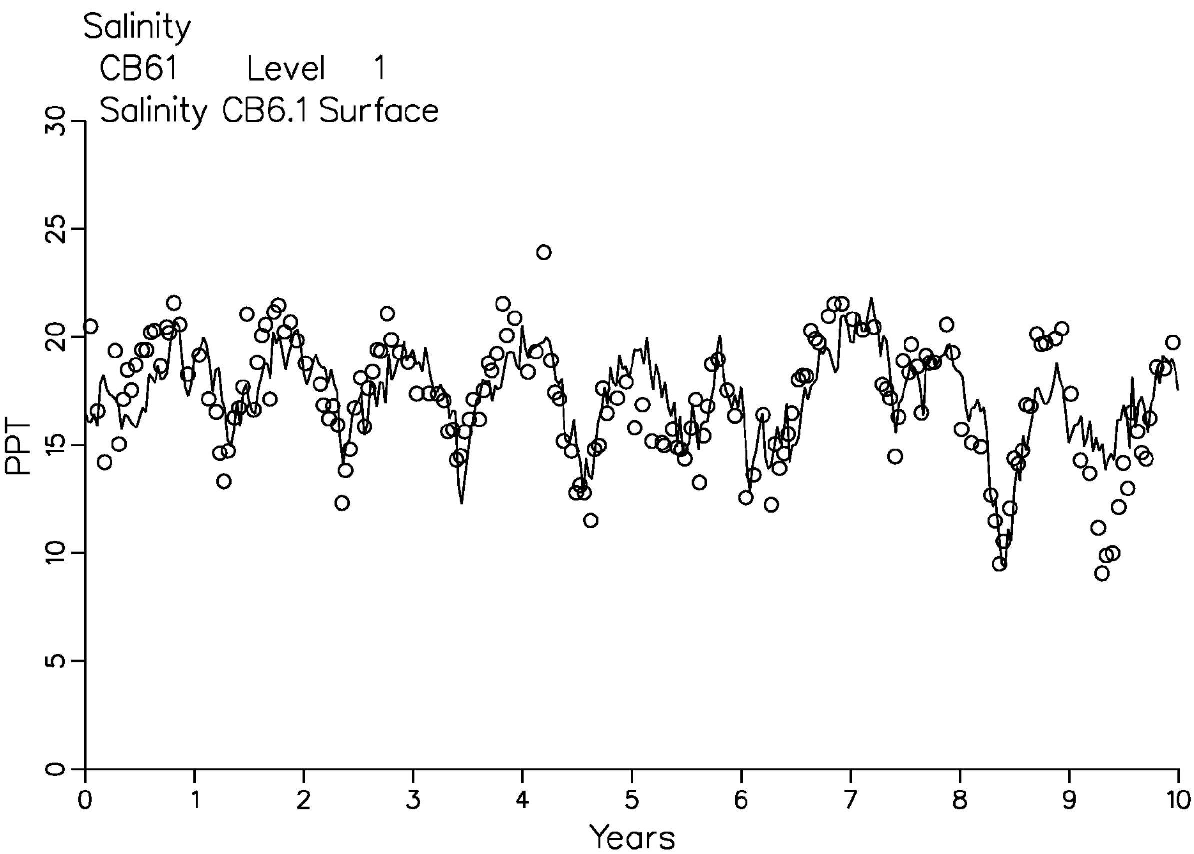

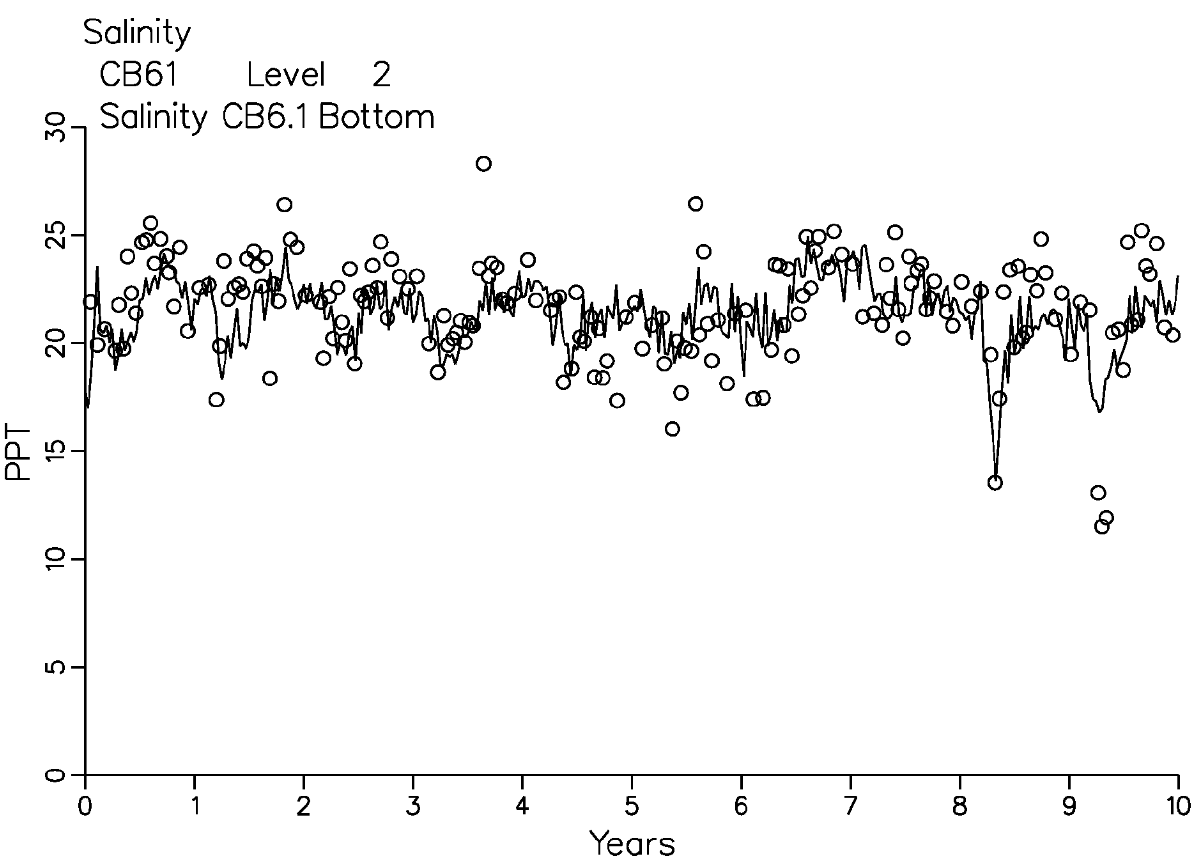

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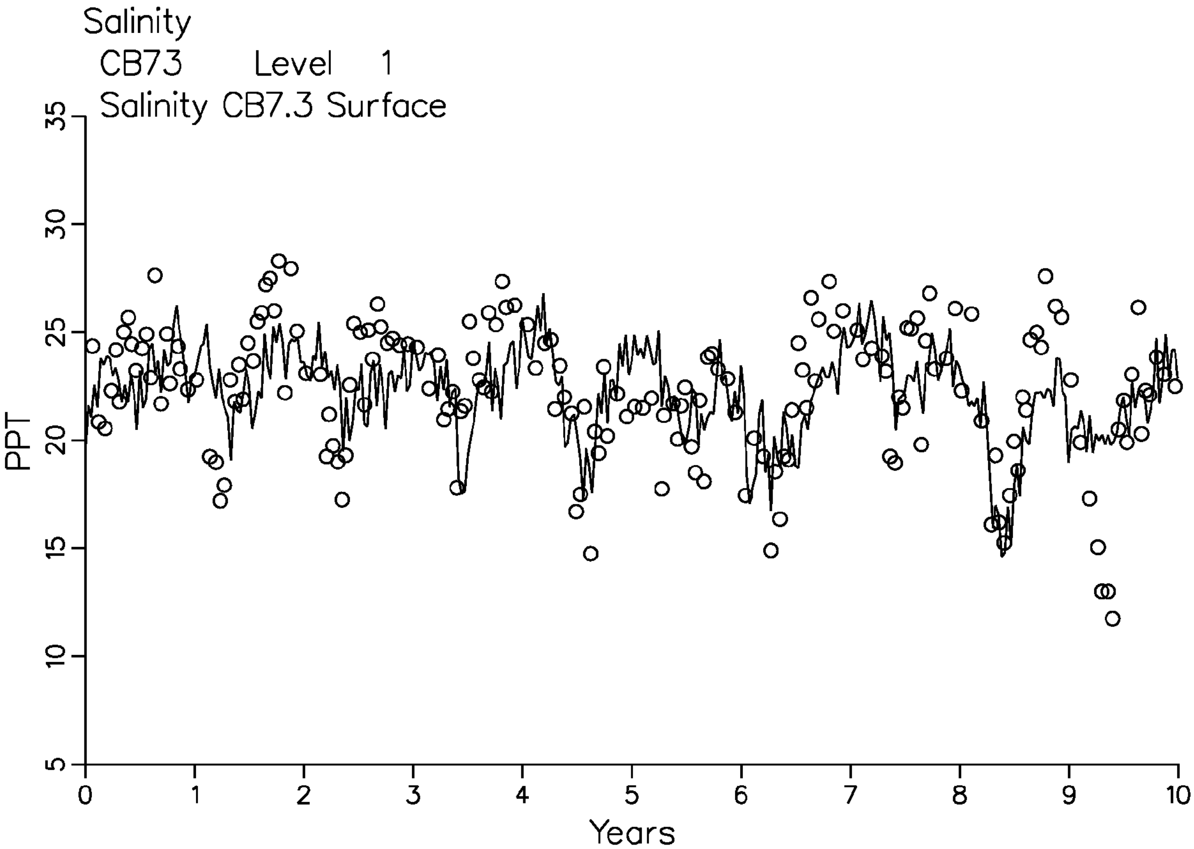

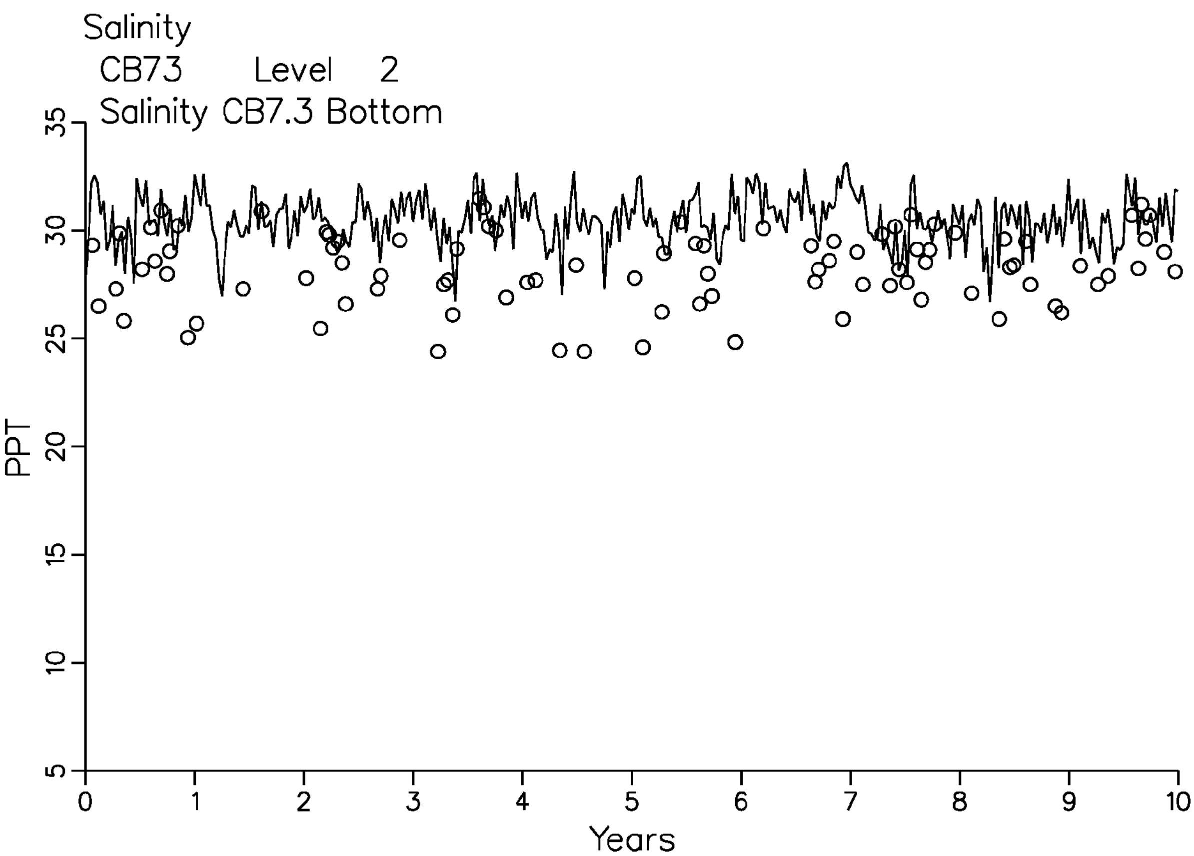

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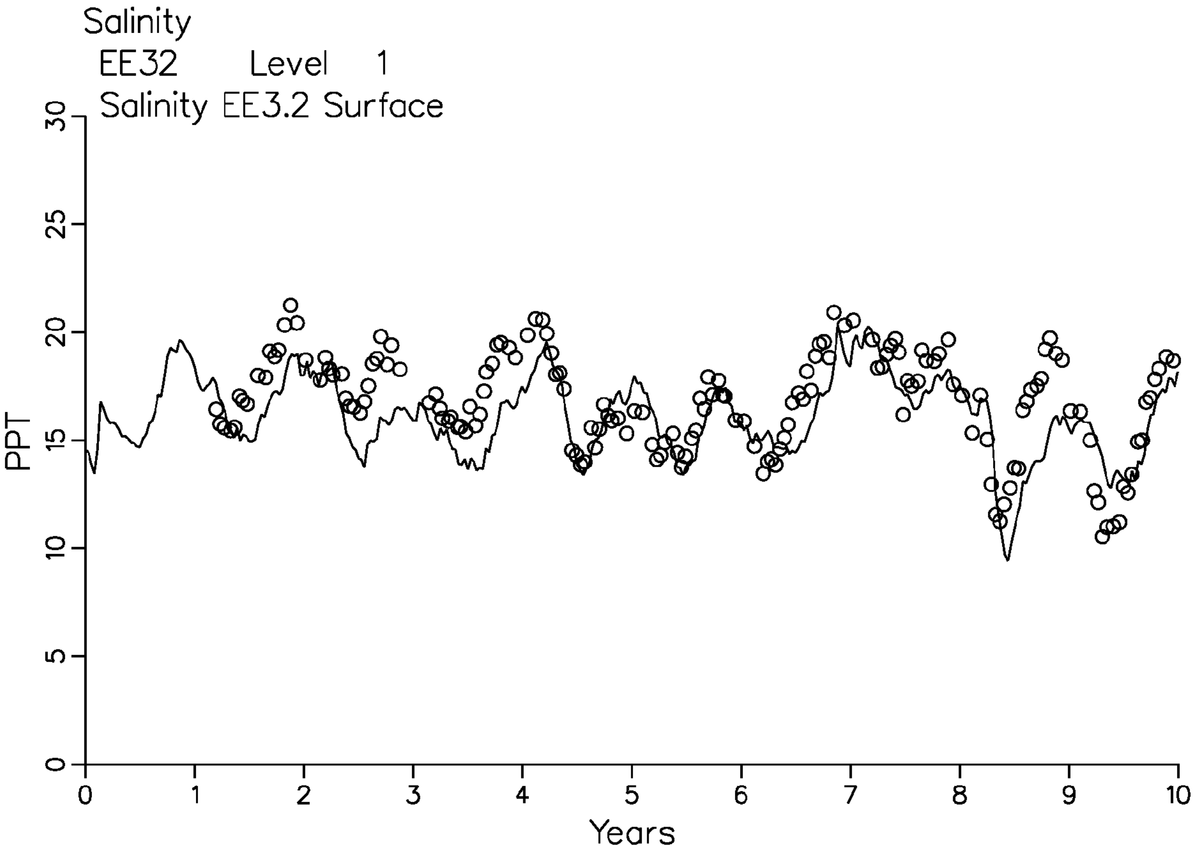

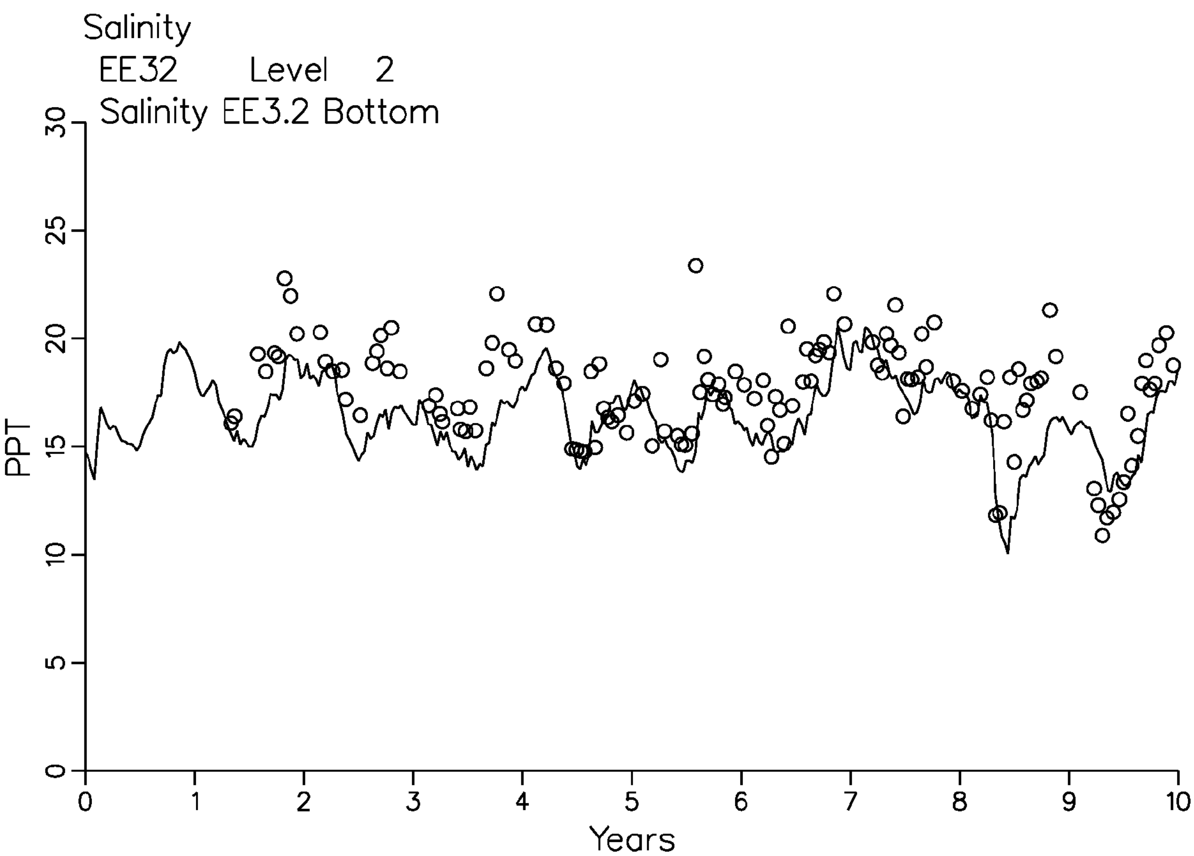

We recognize that our recommendation that use of the water quality model as a management tool should be suspended has serious implications, and we do not make it lightly. In order to give the management community a sense of the depth of our concern, we provide more detail with regard to three specific areas: Salinity Distribution, Primary Production, and Nutrient Uptake and Oxygen consumption Rates.

Primary Production and Dissolved Oxygen

Is Chesapeake Bay an Estuarine Desert?

After repeated requests, we were provided with model calculations of annual net primary production by the phytoplankton at 12 locations in Chesapeake Bay for each of ten years (1985-1994). Six stations are located along the main stem of the bay and there are three along the length of each of the Patuxent and Potomac River tributary estuaries. Annual primary production is apparently not routinely computed or compared with measurements in spite of the fact that biological carbon fixation by the phytoplankton is the dominant source of the organic matter that supports bay food chains and provides the substrate for respiration that can lead to hypoxic and anoxic bottom waters.

It is immediately apparent that the model seriously under computes the amount of organic matter produced in the real bay (Table 1). In the most productive mid-regions of the bay, the amount of carbon fixed in the model averages only about 50% of that measured by the monitoring program. In the productive lower region of the Patuxent and the Potomac tributaries, the amount of organic carbon supplied in the model averages only 25-30% of that measured in the real bay. An inspection of Table 1 also shows that the level of primary production in the model is relatively uniform along the axis of the bay in contrast to the measured data which show a region of much higher production in mid-bay. The year-to-year variation over the ten years from 1985 – 1990 is also greater in the measurements than in the model, and the most productive model year during this period was still lower than the least productive measured year in most of the mid and lower bay (Table 2).

Table 1

Comparison of primary production by phytoplakton in Chesapeake Bay during 1985-1994 as calculated by the water quality model and as measured by the monitoring program. Values are the mean ± 1 S.D. for ten years.

Main Stem of the Bay

Station	Model[1]	Station	Measured[2]	Ratio: Measured/Model
2.2	132 ± 31	2.2	171 ± 79	2.29
3.3	228 ± 37	3.3	407 ± 97	1.78
4.2C	207 ± 30	4.3C	411 ± 113	1.98
5.2	200 ± 16	5.2	411 ± 113	2.05
6.2	123 ± 15	6.1	284 ± 126*	2.31
7.2E	118 ± 13	7.3E	213 ± 110*	1.81

Potomac River Estuary

Station	Model[1]	Station	Measured[2]	Ratio: Measured/Model
XFB 2470	168 ± 65	XEA 6596	337 ± 159	2.00
RET 2.4	147 ± 53	XEA 1177	181 ± 85	1.23
LE 2.2	177 ± 30	MLE 2.2	556 ± 147	3.14

Patuxent River Estuary

Station	Model[1]	Station	Measured[2]	Ratio: Measured/Model
TF1.7	102 ± 57	PXT 0402	347 ± 87	3.40
RET 1.1	202 ± 56	XED 4892	217 ± 74	1.07
LE 1.3	133 ± 26	XDE 5339	503 ± 117	3.78

[1]Computed values for 1985-1994 provided 9/30/99 by Carl Cerco, USACE Vicksburg, MS.
[2]Monitoring data for Maryland 1985-1996 provided by Peter Tango, MD Dept. Natural resources. Lower Bay data (*) from Marshall and Nesius (1996) for 1990-1993 only.

Table 2

Range and coefficient of variation (S.D./ X 100) in annual primary production in the mid-bay region of Chesapeake Bay during 1985-1994 as computed by the water quality model and measured by the monitoring program. Units are g C m^{-2} y^{-1}. See Table 1 for sources.

Station	Model		Measured	
	range	cv, %	range	cv, %
3.3 C	172 – 283	16	245 – 560	24
4.2C	145 – 256	14	280 – 640	27
5.2	175 – 221	8	310 – 795	27

Because the bay monitoring program measures phytoplankton primary production using a ^{14}C uptake approach that is apparently of long standing in Chesapeake Bay (Walter Boynton, University of Maryland, personal communication) but different from other commonly used oceanographic techniques, there have been some concerns that the monitoring data consistently overestimate production. Comparison of the monitoring data with 24 h light-gradient ^{14}C uptake measurements reported by Malone et al. (1988) suggest that this is not the case. Their measurements were made during February – October 1985 and 1986 along a transect in the main stem off the Choptank – Patuxent rivers. If we assume that the average daily production during the missing months of November – January was equal to the low rates they measured in February – April, the Malone et al. (1988) data give annual production of 620 g C m^{-2} y^{-1} in 1985 and 415 g C m^{-2} y^{-1} in 1986. Even if we assume there was no production during November – January, their measured values give 580 and 360 g C m^{-2} y^{-1}, respectively. These results are consistent with the level of production reported by the monitoring program in this region of the bay (Table 1).

Additional evidence consistent with the high level of production reported by the monitoring program is provided by a recent assessment of average primary production by phytoplankton along the entire main stem of Chesapeake Bay developed by Larry Harding (University of Maryland) and colleagues. They based this analysis only on long-term light gradient ^{14}C uptake measurements. Their results show a 12-year (1982, 1987, 1989 – 1998) mean of 330 ± 74 (S.D.) g C m^{-2} y^{-1}, with a range from 225 –450 g C m^{-2} y^{-1}, values clearly much higher than computed by the model (Table 1). We have also computed a very rough area-weighted estimate of main stem production using the monitoring data from only nine stations during 1990 – 1993. While the agreement between our rough estimates from the monitoring program data and the results of Harding and colleagues is not good, there is no indication that the monitoring program technique consistently overestimates main stem production (Table 3). A more detailed, and rigorous, and well documented intercomparison of primary production from Chesapeake Bay is clearly needed, but the important point here is that virtually all the measurements show that the model seriously undercomputes the production of organic matter in the bay.

Table 3

Comparison of the area-weighted mean annual primary production (^{14}C uptake) in the main stem of Chesapeake Bay using measurements from the bay monitoring program and provided by Larry Harding and colleagues at the University of Maryland using 24 h light gradient incubations.

	Production, g C m^{-2} y^{-1}	
Year	Monitoring Program[1]	Harding et al. (in prep.)
1990	280	395
1991	395	340
1992	350	225
1993	490	265

[1]Monitoring data for stations CB1.1, 2.2, 3.3C, 4.3C and 5.2 provided by Peter Tango, MD Dept. Natural Resources. Stations 6.1, 6.4, 7.3E, and 7.4 taken from Marshall and Nesius (1996). The monitoring data were roughly area-weighted by assigning stations to areas of the main stem given in Cronin (1971) as follows:

segment (n mi)	station(s)	segment (n mi)	station(s)
0-10	7.4	75-105	4.3C
10-30	6.4+7.3E	105-140	3.3
30-50	6.1	140-150	2.2
50-75	5.2	150-155	1.1

Overall, numerous studies by the Bay Program and others over the past 20 years have shown at least three very important things about phytoplankton production in the real Chesapeake Bay — it is high, it is concentrated in the mid-bay region, and it is quite variable from year-to-year. In sharp contrast, phytoplankton production in the model bay is low, relatively constant along the main axis, and relatively constant from year-to-year (Fig. 1). The model bay is a dull, undynamic place running on a level of primary production similar to that found in that great "ocean desert", the Sargasso Sea, where recent measurements have shown primary production rates of 145 g C m^{-2} y^{-1} (Lohrenz et al. 1992).

But the Dissolved Oxygen Simulations Look So Good!

During discussions with various members of the modeling group and some managers, we have been asked why we were so concerned by the low primary production rates in the model when it appeared to them that the model computed levels of dissolved oxygen in the bottom water that agreed well with measurements. Let us accept their view of the good agreement, though we have not seen the evidence. The verification runs we have been shown depict annual cycles over ten years and do not focus on the details of summer, when it is most important to get the oxygen right. In any case, the fact is that if the model is computing oxygen levels in the bottom water of the model bay that match the oxygen concentrations in the bottom water of the real bay where the organic input from primary production is 2-3 times greater, there must be one or more other processes in the model that are also very wrong to compensate for the low organic supply in the model. There are numerous possibilities — respiration may be too low in the surface water and/or too high in the bottom water, the flux of organic matter through the pycnoclyne may be too high, oxygen flux across the pycnoclyne may be too low, etc. The inescapable conclusion, however, is that at least two fundamental ecological processes are very wrong in the current water quality model and both are involved in a crucial way with the ability of the model to relate nutrient inputs to hypoxia and anoxia. Moreover, assuming the nutrient inputs to the model are correct, the overall relationship between nutrient load and primary production in the model can not be correct, since current loads result in less than half the real production.

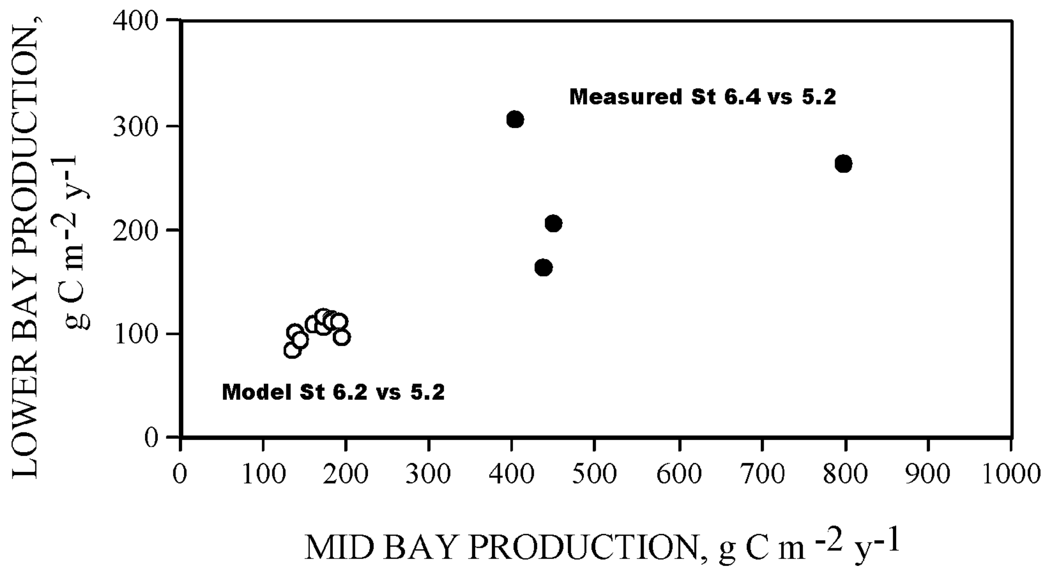

Figure 1. The relationship between phytoplankton primary production in middle (station 5.2) and lower (station 6.4) Chesapeake Bay as measured by the monitoring program and as computed by the water quality model. Lower bay measurements are from Marshall and Nesius (1996) for 1990 – 1993. Model calculations are for 1985 – 1994.

In short, the model does not appear to capture the basic biological dynamics of the bay. In our view, it has no credibility when used in its present form to relate changes in nutrient input to bottom water oxygen concentrations.

This conclusion does not, as some have claimed, simply reflect a bias of academic scientists who do "ecosystem models" against engineers and "engineering models". There is no such thing as an "engineering model" of Chesapeake Bay nutrient-oxygen dynamics. It may, perhaps, be reasonable to think of the hydrodynamics model as an "engineering model", but in a system where the great majority of the oxygen consumption is based on *in-situ* production of organic carbon, you have to have an ecosystem model and it has to get the biology and ecology much closer than a factor of 2 or 3 if the model is going to be credible and of practical value. The fact that the model maintains mass balances is laudable, but it must begin with an accurate input of organic carbon and then stay within the constraints of stoichiometry and mass balance for carbon, oxygen, nitrogen, and phosphorus.

References - Chesapeake Bay

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Appendix C –Nutrient utilization and respiration in the Chesapeake Bay Model.

Introduction. The most recent version of the Chesapeake Bay Model was optimized to fit observed phytoplankton biomass observations and water quality properties, but was not fitted to primary production nor nutrient recycling processes. Both this Report (Appendix B) and Cerco (1999) show that the model tends to underestimate primary production in the light-replete, nutrient-limited mid- and lower reaches of Chesapeake Bay. It may not be possible to obtain satisfactory, biologically realistic parameter sets which simultaneously optimize for all key model state variables and rate processes (Evans, 1999); yet we still wish to "get models right for the right reasons." This aim is especially critical when models have more than academic interest, and when model reliability is needed to support management applications. The bay Model provides the best and most widely known example of this need. In order to gain further insight into the processes supporting primary production in the Model, and perhaps to understand how it underestimates primary production, we examine model outputs related to nutrient (nitrogen) utilization and regeneration (respiration).

Background. Primary production in estuaries can be limited by the supply of either nitrogen or phosphorus, with the limiting species shifting in space and time (Malone et al., 1988; 1996). Although growth rates in spring may be limited by phosphorus, biomass accumulation and primary production are controlled by dissolved inorganic nitrogen (DIN) supply throughout the mid- and lower Bay (Malone et al., 1996). In the open sea, remote from benthic and terrestrial nutrient supplies, primary production is supported by exogenous, or "new" nitrogen, largely deepwater nitrate (NO3), and regenerated forms (ammonium, NH4, and urea) supplied by heterotrophic respiratory processes (Dugdale and Goering, 1967). The relative absence of "new" NH4 (e.g., in rainwater) and regenerated NO3 (e.g., from nitrification) makes it easy to measure the balance of new and recycled nutrients supporting primary production in the sea. The distinction is important because only exogenous inputs support biomass accumulation, export, sedimentation and fisheries (Eppley and Peterson, 1979). This identity is true in estuaries also, but the nutrient regime is more complicated. Ammonium is supplied in riverine inputs and by regeneration from sediments as well as from *in situ* processes in the water column, and *in situ* supplies of nitrate from nitrification can also be significant. However in Chesapeake Bay, both ammonium and nitrate are relatively depleted in the mid and lower Bay surface euphotic layer, downstream of the principal freshwater inputs and isolated from sediments by the summer halocline (Malone et al., 1986). For example, McCarthy et al., (1977) showed that over most of the year throughout the Bay, standing stocks of DIN are insufficient to support a single doubling of the particulate N. In these reaches, especially in summer, production is still largely dependent on *in situ* nitrogen recycling in the upper water column.

A detailed view of nitrogen dynamics in Chesapeake Bay was provided by McCarthy et al., (1977). They showed that in Chesapeake Bay, like the open sea, phytoplankton have a very great preference for reduced forms of N (NH4, urea) throughout the Bay, even when NO3 is abundant, as in the upper Bay. The preference of a given nutrient species is expressed as the Relative Preference Index (RPI):

$$RPI_{NO3} = \frac{\left[\dfrac{V_{NO3}}{\Sigma V_i}\right]}{\left[\dfrac{[NO_3]}{\Sigma[N_i]}\right]}$$

where V_i is the utilization rate for the i-th N species and $[N_i]$ is its concentration (availability). The summations are over all N species (NO3 and NH4 in the Bay Model). If the fraction of total uptake by NO3 is equal to its proportion of all nitrogenous nutrients in the water, the RPI will be 1. Thus RPI provides a useful qualitative and quantitative index of ecosystem performance in supply and utilization of limiting nutrients. McCarthy et al (1977) showed that over most of the Bay, RPI for NH4 was always greater than 1, ranging ca. 1.5 – 60, whereas RPI for NO3 was less than 1 in all but 3 of 36 cases. In other words NH4 was the preferred form of nitrogen for phytoplankton even when its concentration was less than 10% of the nitrate stock. RPI's for NO3 and NH4, which constitute the total N supply in the Bay Model, can be easily compiled from model output. McCarthy et al. (1977) provides a comprehensive data set on RPI for comparison.

Nutrient regeneration processes include excretion by grazers, decomposition of organic particulate and dissolved matter by protozoans and bacteria, and microbial ammonification/ nitrification and release from sediments. The current Model includes just rudimentary representations of these processes. Further, there are few data sets, even in the Bay Monitoring Program, on these processes. Thus comparison of observed vs modeled recycling processes is difficult, if not impossible. The single exception is respiration in the water column and sediments. Most nutrient regeneration is linked physiologically to respiratory processes and there is a good data set available for comparison with model output. Early representations of Chesapeake Bay metabolism suggested a preponderance of benthic respiration (Officer et al., 1984). Recent observations, including seasonal studies at stations in the upper-, mid- and lower Bay, demonstrate that planktonic respiration usually exceeds benthic respiration (including sulfate reduction) by a factor of 2-3 or more (Kemp et al., 1992, 1997). Further, gross primary production exceeded the total respiration integrated over the whole Bay and over the annual cycle by about 3%. Chesapeake Bay was slightly net autotrophic in 1990-92. Ratios of GPP:Respiration and planktonic:benthic respiration provide further indices of system performance for model-data comparisons.

Model Output and Observed Data. Model output was kindly supplied in Excel by Carl Cerco as quarterly (seasonal) averages over the 10-year 1985-94 standard model run of the CBM at 3 stations corresponding to the upper-, mid- and lower Bay stations from Kemp et al., (1977). Initially the Model reported water column respiration rates which were about 8 times higher than the observations. These were not the values actually computed by the Model, but rather incorrectly reported by the model output. As a result of this review, the model was corrected to report the correctly computed rate values. It was clear, however, that modeled respiration had never been compared with observed values. Water column averaged data were converted to integrals by multiplying by model depths of 5.2, 23.5 and 12.3 m, respectively, for the 3 stations. Oxygen- and carbon-based rates were compared assuming mean PQ and RQ values of 1.0 (Kemp et al., 1997). RPI's for NO3, NH4 were calculated on data as supplied in quarterly averages, which undoubtedly introduces some bias when nutrient concentrations are near seasonal extremes. Raw data on observed respiration were kindly supplied by WM Kemp and Erik Smith (Horn Point Lab). (see Figure legends).

Results and Comparisons.

Nutrient utilization. Model nutrient concentrations, from which RPI's are calculated, are shown in Fig. 1. Nitrate is highest in the upper Bay, reflecting the Susquehanna River source, and downstream utilization. Ammonium is more uniform throughout the Bay, as a result of *in situ* sources via local regeneration processes. Uptake rates do not show any strong or obvious relationship to ambient concentrations (Fig. 2) in the model. Low NO3 uptake at the highest concentrations indicates the effect of light limitation in upper bay areas. In the model NO3 was generally 50-90% of the DIN pool, except in the lower bay (Table 3), and it contributed 10-60% of the total N utilization (Tables 1-3). While the relative sizes of the pools in the model matched observations, the relative utilization differed greatly (Table 4). The relationship between the fractional NO3 uptake and ammonium concentration is related to position in the Bay: in the upper Bay, [NH4] seems to inhibit NO3 uptake, but [NH4] and NO3 uptake rates covary directly in the mid- and lower bay. This pattern contrasts sharply with that actually observed in the Bay by McCarthy et al (1977), where NO3 was only an important contributor to phytoplankton nutrition at the lowest [NH4] (Fig. 3 dashed lines).

Model RPI's for NH4 and NO3 are greater than 1 and less than 1, respectively, as observed in the Bay (Fig. 4, Tables, 1,2), but the range of values is much reduced compared to observations (Figs. 4-6). RPI for NH4 was strongly correlated with [NO3] (Fig. 5), a relationship which is quite weak in the observations (Fig. 5, lower panel). Model RPI's vary much less than the observations, which range up to over 60 (Fig. 5, lower). To some extent this attenuation might be a consequence of the quarterly averaging of model data supplied for this analysis. Modeled RPI's for NO3 also differ significantly from observations (Fig. 6), being generally higher over the full concentration range for NH4 and total-N.

Thus in the model, phytoplankton preference for NO3 is stronger, and the preference for NH4 is weaker than the respective observations, by as much as an order of magnitude. This may have several implications for model performance. In the upper Bay, where the model tends to reproduce primary production observations the best, phytoplankton have a much stronger preference for NO3 than is actually observed. The match between modeled and observed PP may be driven by over-reliance on plentiful NO3 supply in that region. In the lower Bay, where the agreement with observed PP is weakest, enhanced NH4 utilization could help close the gap. ***Overall, model PP relies much more on exogenous NO3 than does the real Bay. Since oxygen depletion and harvesting of living resources depends entirely (in the long term) on new production supported by riverine N, it seems important to improve this aspect of Bay model operation.***

Respiration. To gain insight into nutrient resupply processes we examined respiration in the Bay model. Plankton respiration was within a factor of two of the observed values, but about

30-40% low in the mid and lower bay, especially in summer (Fig. 7, Table 5). In contrast, benthic respiration (sediment oxygen consumption only) was close to the observed values (Fig. 8, Table 5) Plankton respiration exceeded benthic respiration in the model as in the observations (Table 5). Overall, sediment plus water column respiration is lower in the model than the observations, suggesting the insufficiency of nutrient regeneration implied by the RPI analysis. Another view of the metabolic relationships in the model can be obtained through comparison of respiration with gross primary production rates (GPP, Table 6). In the Bay itself, there is a slight (3%) excess of GPP over total respiration (Kemp et al., 1997). Chesapeake Bay may fluctuate around a metabolic P:R balance of 1:1. Simple arithmetic averaging of the monthly observations shows that the lower bay (with the largest area) is nearly balanced, or slightly autotrophic, whereas in the mid- and upper bay respiration exceeds GPP. In the model, the bay is strongly net heterotrophic (P<R) throughout (Table 6), probably due to underestimates of primary production (Table 6 and Appendix B).

Conclusion.

In reality Chesapeake Bay is among the most productive of the worlds estuaries, as a result of efficient recycling and strong algal affinity for regenerated nutrients (NH4, urea). It is a system balanced finely between net production and respiration. Harvests of living resources depend on that balance. The model Bay necessarily has a much simpler ecosystem than the real Bay, so it is unrealistic to demand too close agreement in every aspect of comparison between the two. However our analyses suggest that the Bay Model, although it reproduces biomass, nutrient and oxygen fields well, does a poor job of simulating ecosystem function. Primary production is too low, except in the small area of the upper bay. Respiratory activity is too low, but not sufficiently low to offset the shortfall in primary production. As a consequence the model Bay consumes more organic matter and oxygen than it produces. Perhaps more seriously, the model Bay is too reliant on riverine inputs of NO3, the primary target of waste treatment managers and tributary strategies. ***These problems in representation of ecosystem function point toward potential problems in projecting relationships between changing nutrient inputs, production, oxygen depletion and living resources. Although the model appears to simulate oxygen concentrations rather well, the balance of physical and biological processes generating the oxygen fields may be incorrect. Future work in model refinement should be directed at more ecologically realistic representations of Bay functioning.***

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Table 1. Seasonal and annual averages for nitrogenous nutrient concentration and utilization in Chesapeake Bay Model (Upper Bay Station).				
Average	**Nutrient**	**% of Σ N Conc**	**% Σ N Utilization**	**RPI**
Winter	NO3	0.94	0.33	0.35
	NH4	0.06	0.67	12.1
Spring	NO3	0.95	0.43	0.45
	NH4	0.05	0.57	12.2
Summer	NO3	0.91	0.46	0.51
	NH4	0.09	0.54	6.7
Autumn	NO3	0.89	0.43	0.49
	NH4	0.11	0.57	6.3
Annual	NO3	0.92	0.41	0.45
	NH4	0.08	0.59	9.26

Table 2. Seasonal and annual averages for nitrogenous nutrient concentration and utilization in Chesapeake Bay Model (Mid Bay Station).				
Average	**Nutrient**	**% of Σ N Conc**	**% Σ N Utilization**	**RPI**
Winter	NO3	0.84	0.52	0.62
	NH4	0.16	0.48	3.5
Spring	NO3	0.91	0.55	0.60
	NH4	0.09	0.45	5.5
Summer	NO3	0.78	0.42	0.53
	NH4	0.22	0.58	3.0
Autumn	NO3	0.56	0.37	0.69
	NH4	0.44	0.63	1.7
Annual	NO3	0.77	0.46	0.61
	NH4	0.23	0.54	3.38

Table 3. Seasonal and annual averages for nitrogenous nutrient concentration and utilization in Chesapeake Bay Model (Lower Bay Station).				
Average	**Nutrient**	**% of Σ N Conc**	**% Σ N Utilization**	**RPI**
Winter	NO3	0.60	0.47	0.81
	NH4	0.40	0.53	1.6
Spring	NO3	0.74	0.50	0.69
	NH4	0.26	0.50	2.3
Summer	NO3	0.40	0.30	0.84
	NH4	0.60	0.70	1.3
Autumn	NO3	0.36	0.29	0.87
	NH4	0.64	0.71	1.2
Annual	NO3	0.52	0.39	0.45
	NH4	0.48	0.61	1.56

Table 4. Annual average for nitrogenous nutrient concentration and utilization in Chesapeake Bay Model (entire Bay). Observations from McCarthy et al (1977) include NO2 and urea.

	Model % Total N conc	**Obs % total N conc**	**Model % total N Util**	**Obs % total N Util**
NO3 (+ NO2)	0.74	0.78	0.42	0.29
NH4 (+ urea)	0.26	0.22	0.57	0.71

Table 5. Planktonic and benthic respiration in the Chesapeake Bay Model and observed values[1].

Region	model (M)	obs (O)	Ratio (M:O)
	$gO_2\ m^{-2}\ d^{-1}$		
Upper Bay			
planktonic (P)	2.02	1.64	1.23
benthic (B)	0.48	0.46	1.04
P:B ratio	4.23	3.57	
total	2.50	2.10	1.19
Mid Bay			
planktonic (P)	4.79	6.72	0.71
benthic (B)	0.60	0.52	1.15
P:B ratio	7.98	12.92	
total	5.39	7.24	0.74
Lower Bay			
planktonic (P)	2.51	4.07	0.62
benthic (B)	0.71	0.62	1.15
P:B ratio	3.52	6.56	
total	3.22	4.69	0.69

[1] Annual averages calculated from quarterly averages over 10 year model run, and over 12 monthly values in Kemp et al., (1997). Benthic values are sediment oxygen consumption only. Original water column values multiplied by depth to obtain integrals.

Table 6. Gross primary production (GPP) and total (planktonic plus benthic respiration (both $gO_2\ m^{-2}\ d^{-1}$) in the Bay Model and observations[2].

	GPP		Respiration		P:R	
	model	**obs**	**model**	**obs**	**model**	**obs**
Upper	2.15	1.00	2.50	2.10	0.86	0.48
Mid	3.51	5.38	5.39	7.24	0.65	0.74
Lower	2.16	5.53	3.22	4.69	0.67	1.18

[2] Annual averages calculated from quarterly averages over 10 year model run, and over 12 monthly values digitized from Figures 3,4,5 in Kemp et al., (1997).

Figure 1. Modeled nutrient concentrations in the Chesapeake Bay Model, standard run, 1985-94.

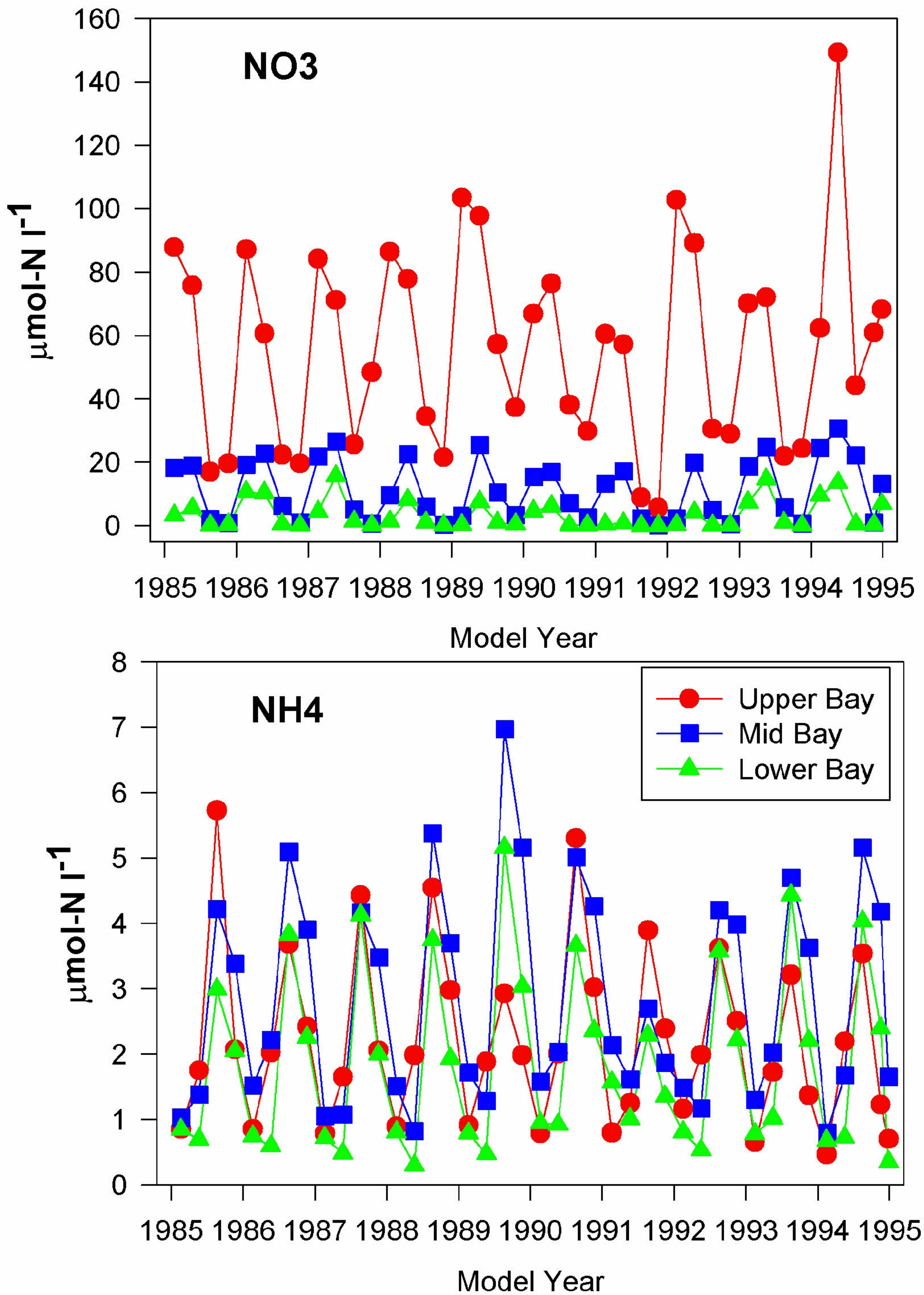
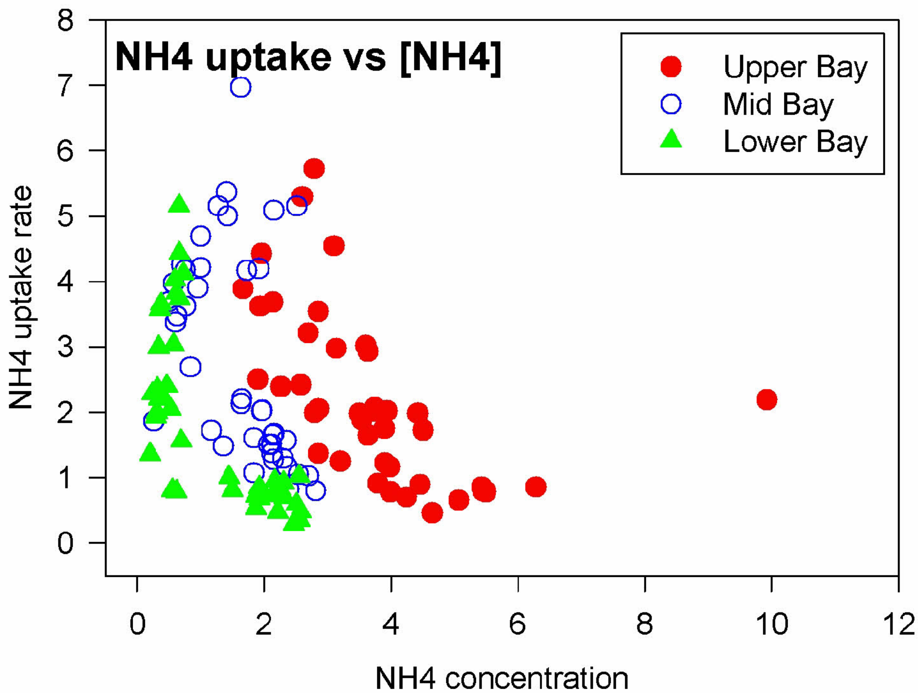


Figure 2. Relationship between nutrient uptake rates and ambient concentrations in the Bay Model.



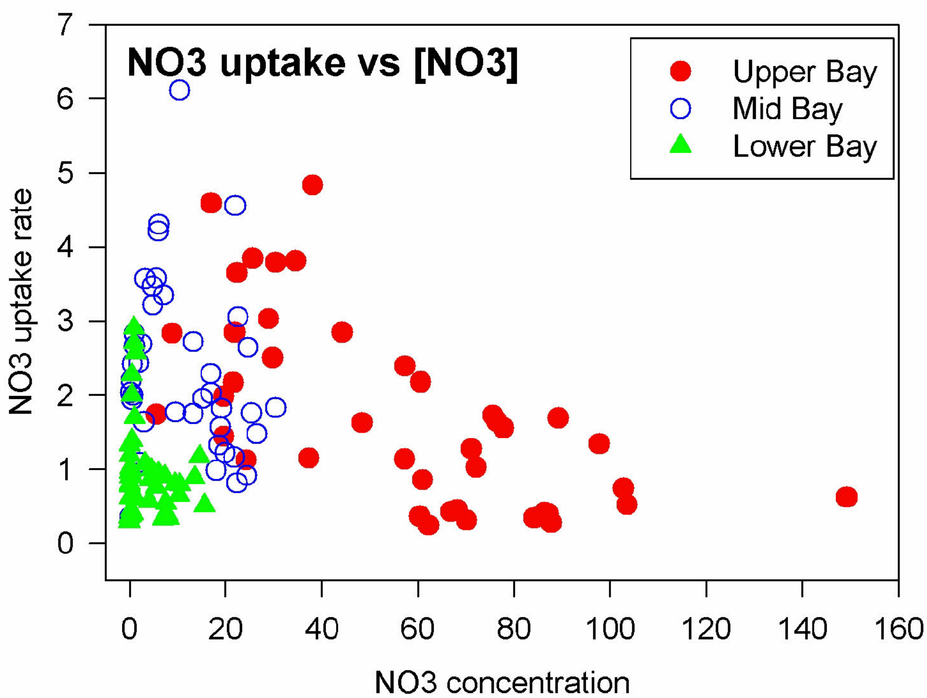
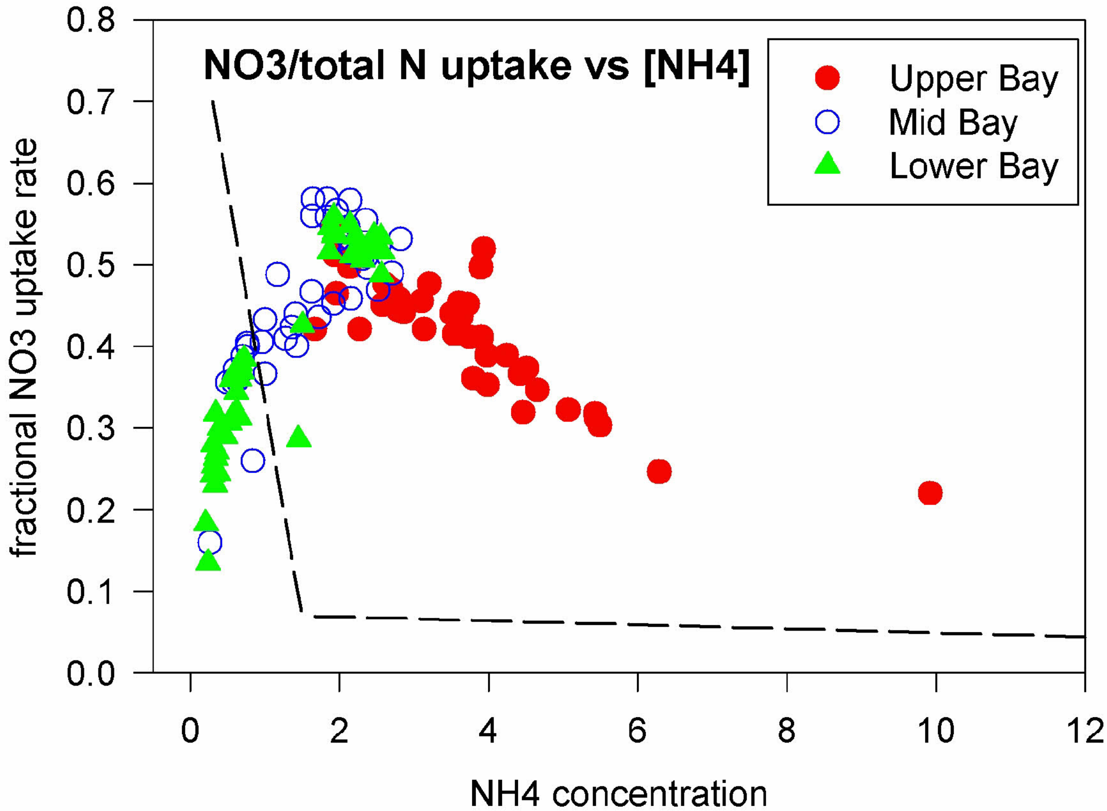


Figure 3. Relationship between ambient ammonium concentration and the fraction of nitrate to total N-uptake in the Bay Model. The dashed line defines the relationship observed in Chesapeake Bay (McCarthy et al., 1977).



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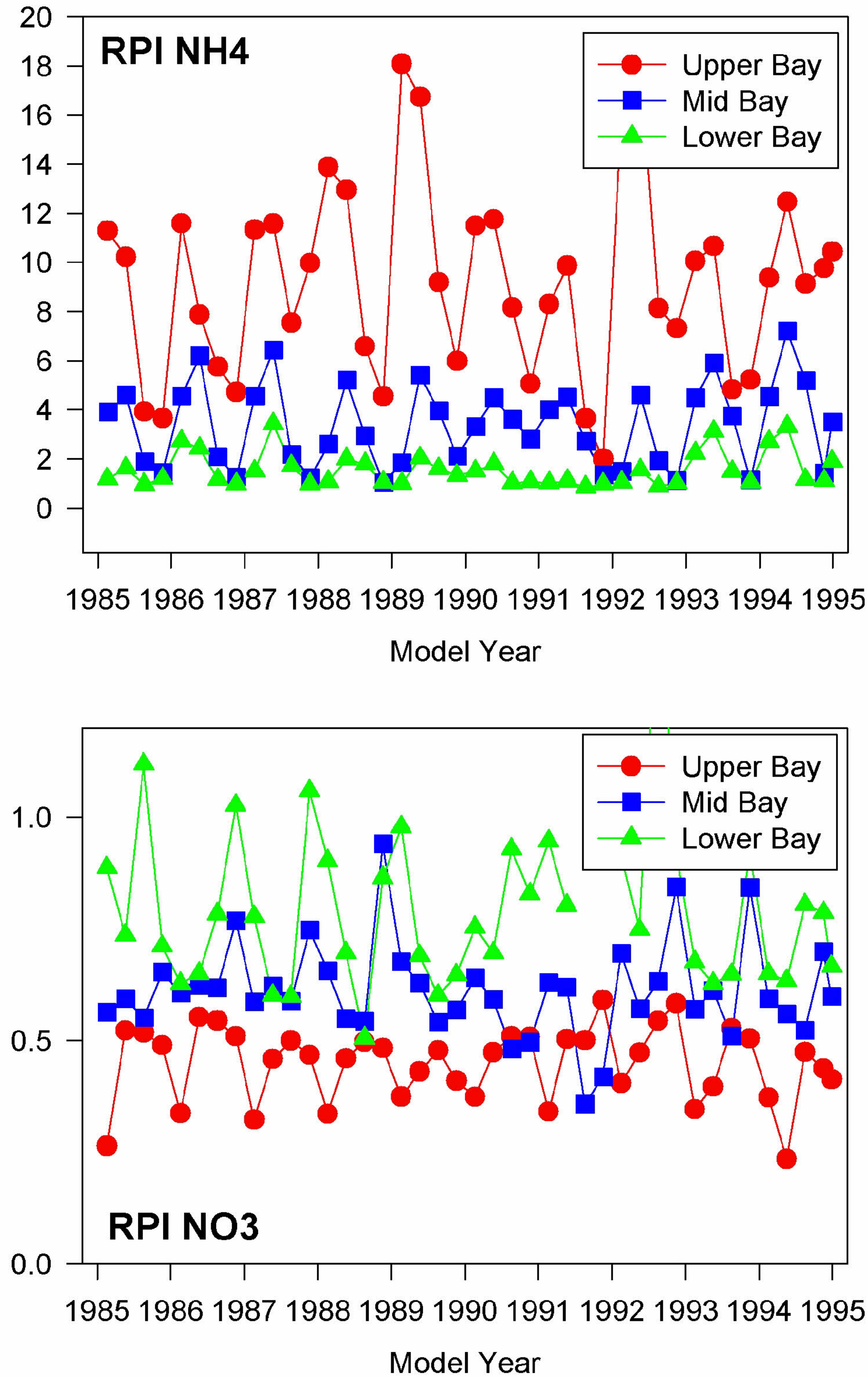

Figure 4. Relative preference indices (RPI, see text for formula) for nitrate and ammonium utilization in the Chesapeake Bay Model.

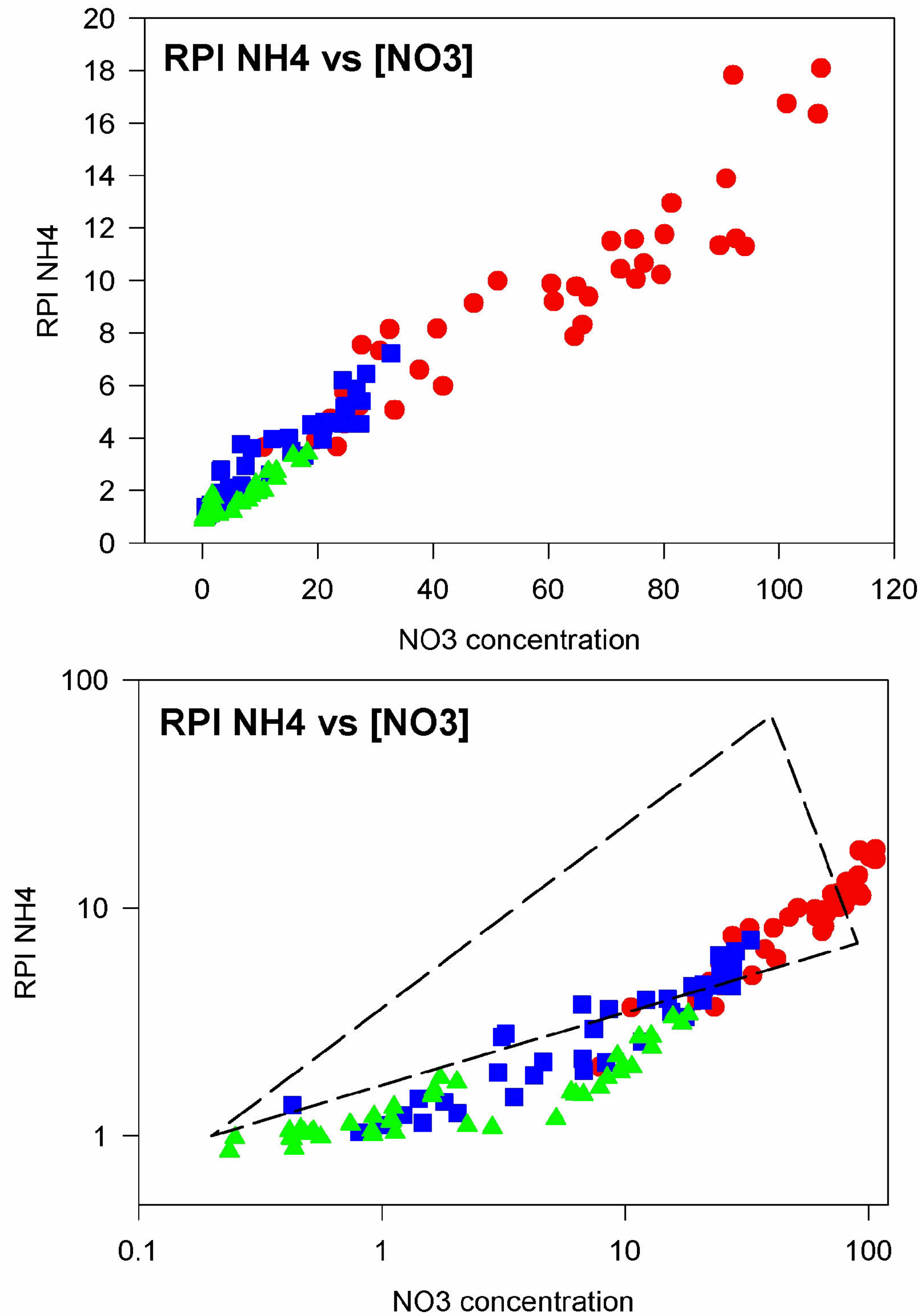

Figure 5. Relationship between RPI for ammonium and ambient nitrate concentration. The triangular region in the lower panel defines the observed data (McCarthy et al., 1977). Note that lower panel in a log-log plot.

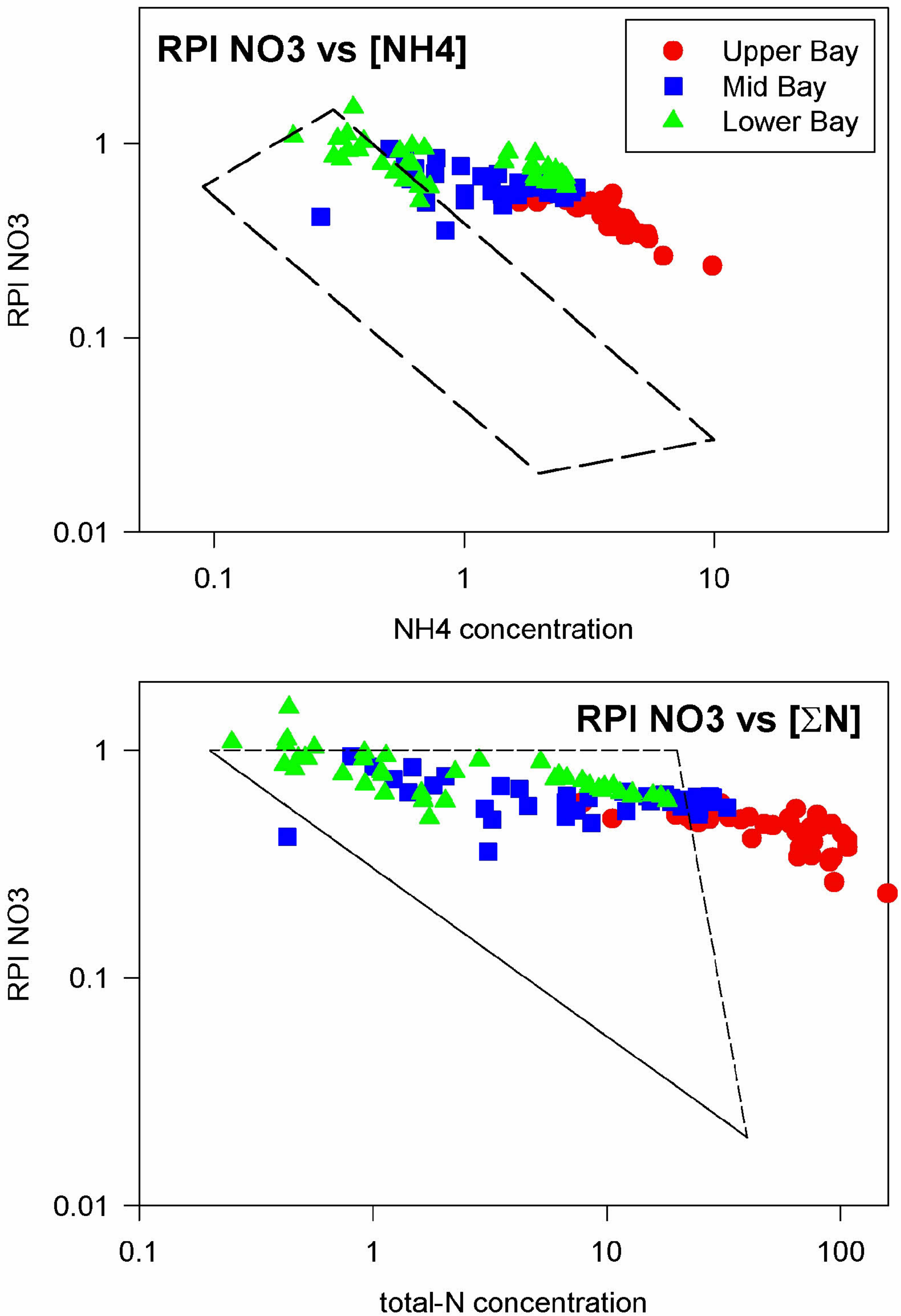

Figure 6. Relationships between RPI for nitrate and ambient nitrate and total-N concentrations. The triangular regions define the observed data (McCarthy et al., 1977). Note: log-log plots.

Figure 7. Plankton respiration in the Chesapeake Bay model (solid circles). Quarterly water column averages (volumetric rates) for years 1985-94 shown as a single composite year. Observations digitized from raw data used to compile Table 1 of Kemp et al., (1997).

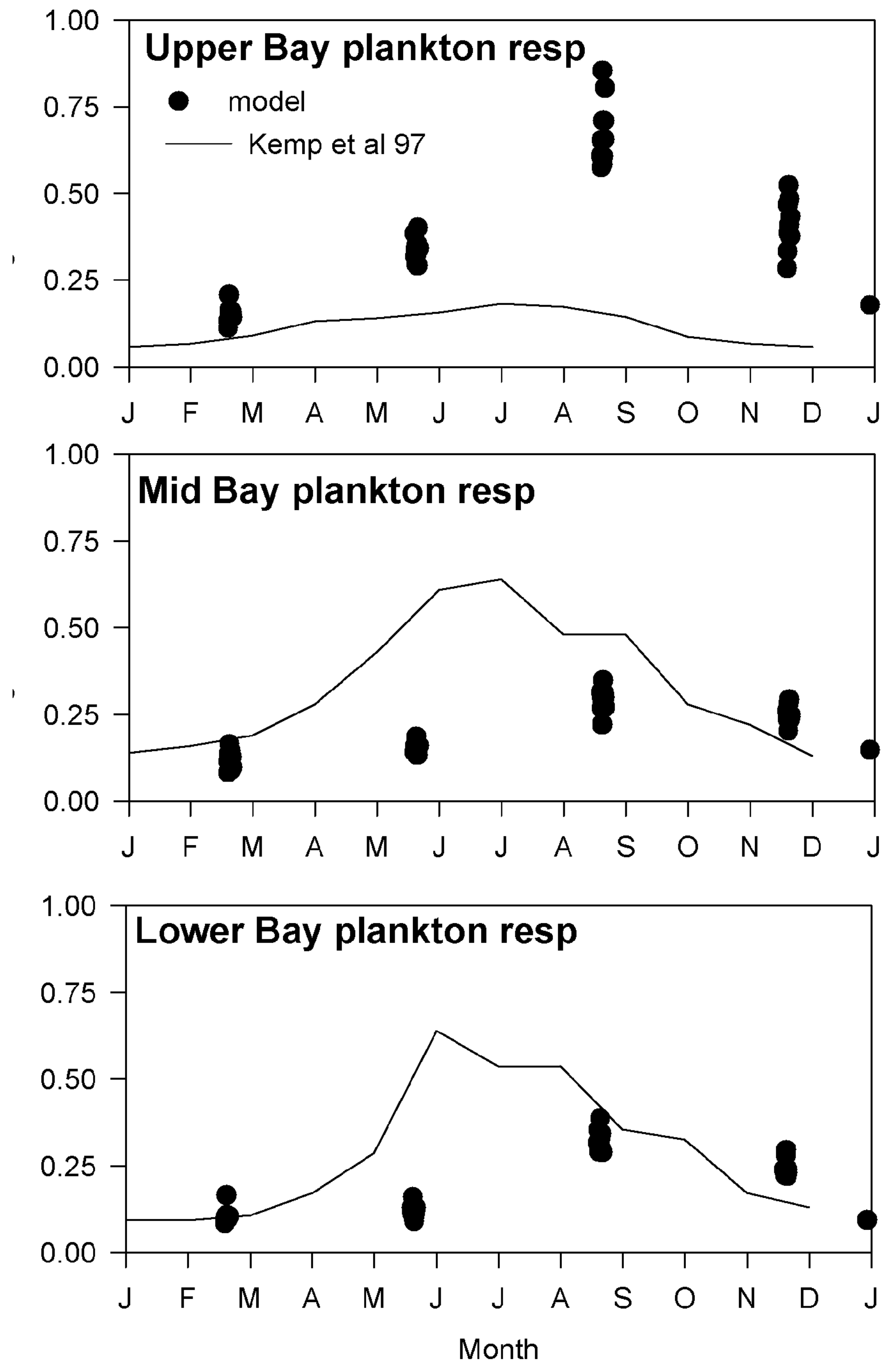

Figure 8. Benthic respiration (sediment oxygen consumption) in the Chesapeake Bay model (solid circles). Quarterly averages (areal rates) for years 1985-94 shown as a single composite year. Observations digitized from Figure 5 of Kemp et al., (1997).

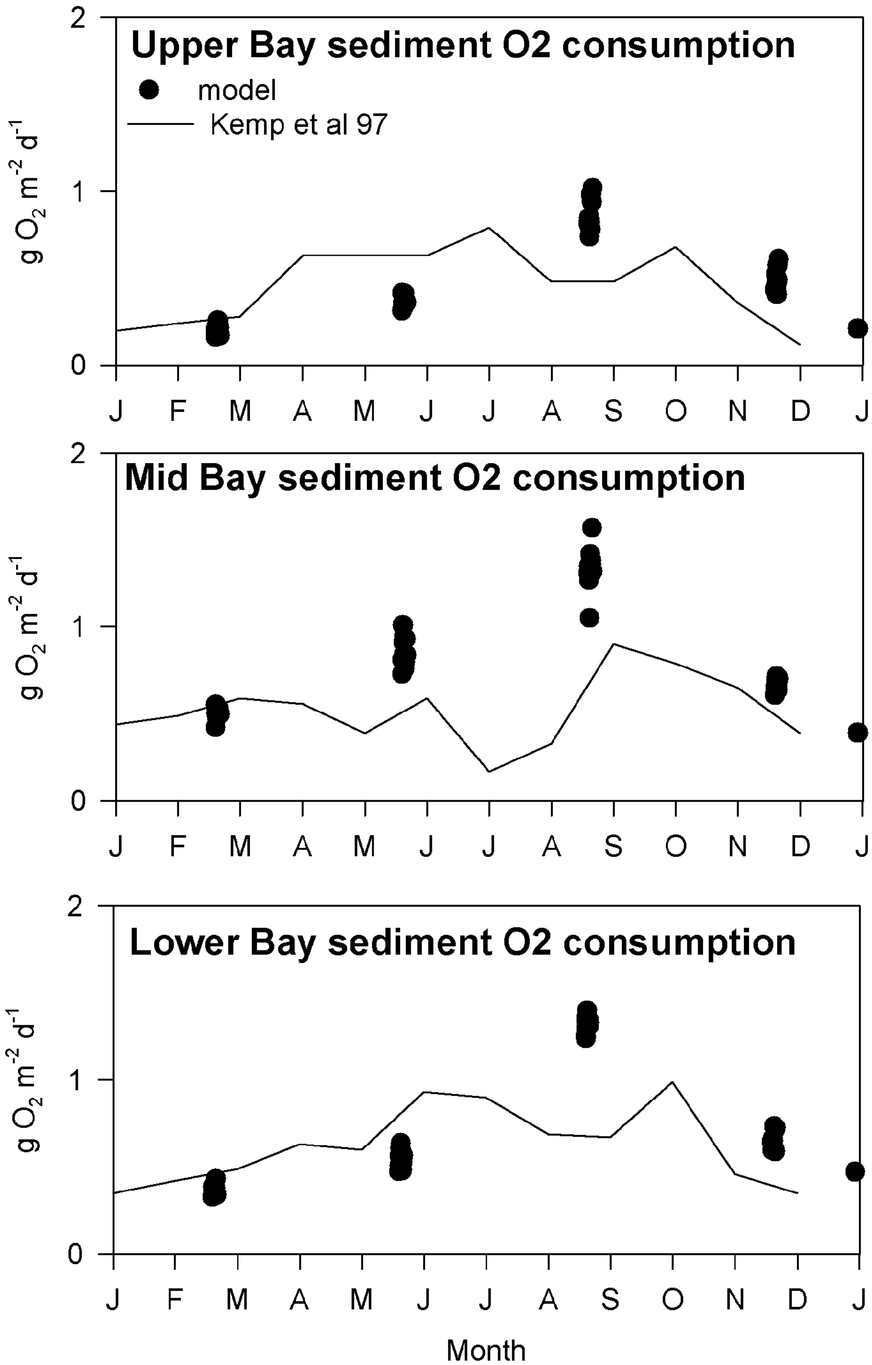

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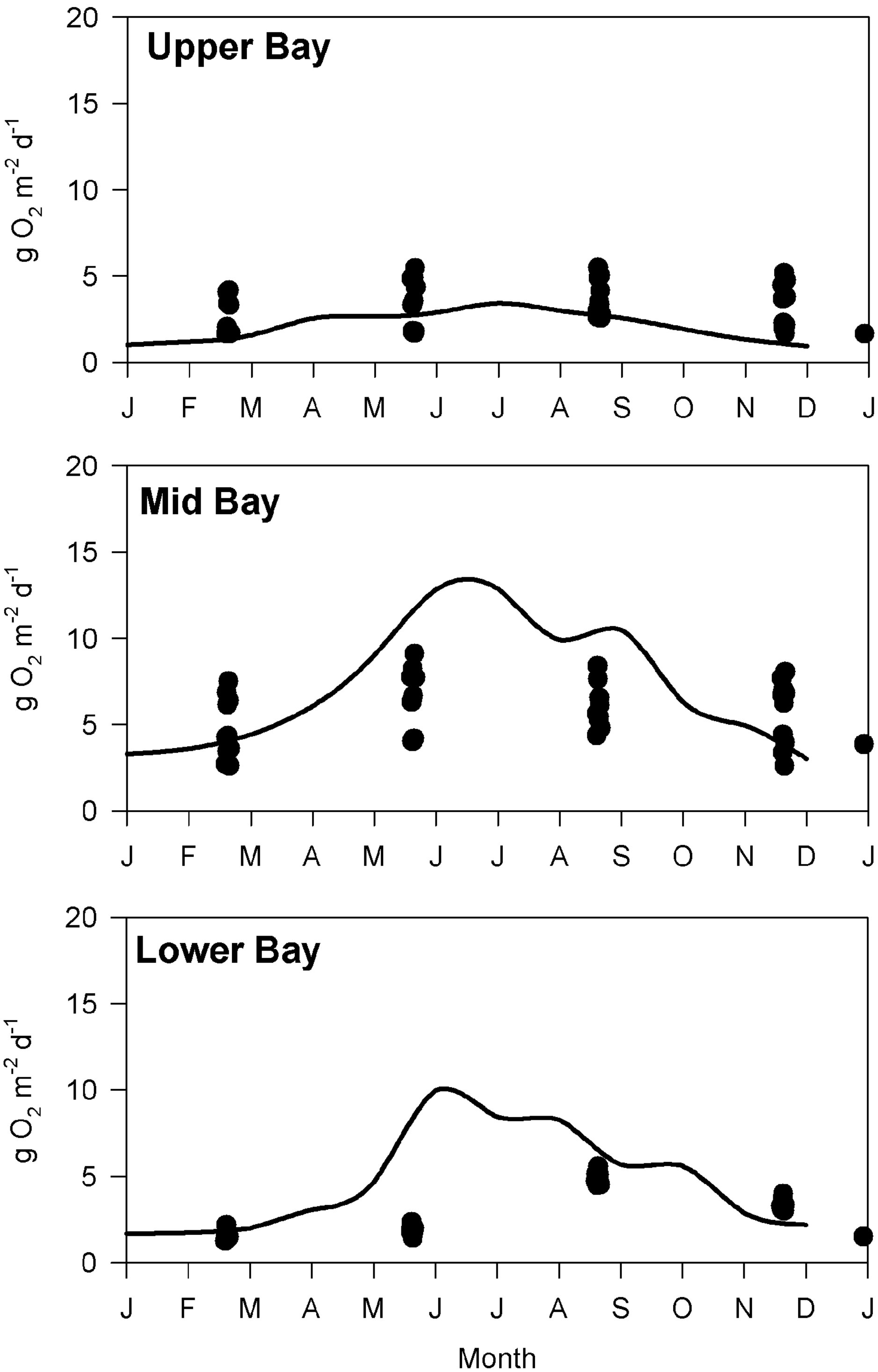
Figure 9. Total water column plus benthic oxygen consumption (circles) in the Chesapeake Bay model. Quarterly averages (areal rates) for years 1985-94 shown as a single composite year. Observations for plankton plus benthic respiration (line) digitized from Figures 4,5 and table 1 of Kemp et al., (1997).



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